



Description

CRYSTALLIZED CYTOPLASMIC TIE2 RECEPTOR TYROSINE KINASE  
DOMAIN AND METHOD OF DETERMINING AND DESIGNING  
MODULATORS OF THE SAME

Technical Field

The present invention relates generally to the structure of the cytoplasmic Tie2 receptor tyrosine kinase domain, and particularly to the structure of the catalytic core, the kinase insert domain and the C-terminal tail of the cytoplasmic Tie2 receptor kinase domain. The invention further relates to methods by which modulators of the cytoplasmic Tie2 receptor kinase domain can be identified.

Abbreviations

ADP	adenosine diphosphate
A-loop	activation loop
AL	activation loop
Ang1	angiopoietin 1
Ang2	angiopoietin 2
Ang3	angiopoietin 3
Ang4	angiopoietin 4
APC	allophyocyanin
ATP	adenosine triphosphate



	BSA	bovine serum albumin
	cAPK	cAMP dependent protein kinase
	CL	catalytic loop
	CTT	C-terminal tail
5	DTT	dithiothreitol
	EGF	epidermal growth factor
	FGF	fibroblast growth factor
	FGFR1	fibroblast growth factor receptor 1
	HEPES	N-2-Hydroxyethylpiperazine-N'-2-ethanesulfonic acid
10	HPLC	high performance liquid chromatography
	Ig	immunoglobulin
	IMAC	immobilized metal affinity chromatography
	IR	insulin receptor
	IRK	insulin receptor kinase
15	KID	kinase insert domain
	kDa	kilodalton(s)
	LCMS	liquid chromatography mass spectrometry
	MS	mass spectrometry
	NBL	nucleotide binding loop
20	NDP	nucleotide diphosphate
	NTP	nucleotide triphosphate
	PAGE	polyacrylamide gel electrophoresis
	PCR	polymerase chain reaction
	PDGF	platelet derived growth factor

	pi	isoelectric point
	PTB	phosphotyrosine binding
	PTK	protein tyrosine kinase
	RMS	root mean square
5	RMSD	root mean square deviation
	RTK	receptor tyrosine kinase
	SDS	sodium dodecyl sulfate
	Sf9	<i>Spodoptera frugiperda</i> 9
	SH2	src homology 2
10	VEGFR1	vascular endothelial growth factor receptor 1
	VEGFR2	vascular endothelial growth factor receptor 2

### Background Art

Growth factors play important roles in the control of cell growth, differentiation, metabolism and oncogenesis, notably through the cellular process of angiogenesis and vasculogenesis. The signals generated by a growth factor are transduced across the cellular membrane by transmembrane receptors specific for the growth factor. The diverse biological effects of growth factors are mediated by a large family of cell surface transmembrane receptors with intrinsic protein tyrosine kinase (PTK) activity. The extracellular portion of receptor PTKs contain the binding site for its particular growth factor/ligand, whereas the tyrosine kinase activity resides in the cytoplasmic portion. Binding of a growth factor to the extracellular domain of this receptor results in autophosphorylation of specific tyrosine

residues in the cytoplasmic domain. These phosphotyrosines either stimulate PTK activity or serve as binding sites for downstream signaling proteins containing Src-homology 2 (SH2) or phosphotyrosine binding (PTB) domains.

Eighteen classes or subfamilies of human receptor PTKs have been identified to date, including the insulin receptor (IR), EGF-receptor, PDGF receptor and FGF-receptor. Ligand-induced dimerization of receptors such as the EGF, PDGF and FGF receptors is thought to be essential for activation. Growth factors such as PDGF are dimeric molecules which, by themselves, are able to induce PDGF-receptor dimerization. However, FGFs are monomeric and are unable by themselves to induce receptor dimerization. Dimerization of FGF receptors is thought to be mediated by FGF in concert with heparin sulfate proteoglycans (soluble or cell surface bound). The identified receptor PTKs have been implicated in a variety of disease states, notably angiogenesis- and vasculogenesis-related conditions.

Both controlled and uncontrolled angiogenesis are thought to proceed in a similar manner. Endothelial cells and pericytes, surrounded by a basement membrane, form capillary blood vessels. Angiogenesis begins with the erosion of the basement membrane by enzymes released by endothelial cells and leukocytes. The endothelial cells, which line the lumen of blood vessels, then protrude through the basement membrane. Angiogenic stimulants induce the endothelial cells to migrate through the eroded basement membrane. The migrating cells form a "sprout" off the parent blood vessel, where the endothelial cells undergo mitosis and proliferate. The

endothelial sprouts merge with each other to form capillary loops, creating the new blood vessel.

It is recognized that angiogenesis plays a major role in the metastasis of a cancer. If this angiogenic activity could be repressed or eliminated, then  
5 the tumor, although present, would not grow. In the disease state, prevention of angiogenesis could avert the damage caused by the invasion of the new microvascular system.

As noted, vasculogenesis and angiogenesis are critical processes in embryonic development as well as in a number of diseases states, including  
10 ischemic coronary artery disease, cancer, diabetic retinopathy and rheumatoid arthritis (Folkman & Shing, (1992) *J. Biol. Chem.* 267: 10931-10934; Risau, (1995) *FASAB J.* 9: 926-933; Pepper, (1996) *Vasc. Med.* 1: 259-266; Kuiper et al. (1998) *Pharmacol. Res.* 37: 1-16; Kumar & Fidler (1998) *In Vivo* 18: 27-34; Szekanecz, et al. (1998) *J. Investig. Med.* 46: 27-  
15 41; Tolentino & Adamis, (1988) *Int. Ophthalmol. Clin.* 38: 77-94). Persistent, unregulated angiogenesis occurs in a multiplicity of disease states, and abnormal growth by endothelial cells and supports the pathological damage seen in these conditions. The diverse pathological disease states in which unregulated angiogenesis is present have been grouped together as  
20 angiogenic-dependent or angiogenic-associated diseases.

While the precise molecular mechanisms that regulate these processes have not been fully elucidated, normal vascular development is known to be dependent on the function of several endothelial specific receptor tyrosine kinases (RTKs) (reviewed in Tallquist et al., (1999) *Oncogene* 18: 7917-7932;

Merenmies et al., (1997) *Cell Growth Differ.* 8: 3-10). These include the Tie RTKs, Tie1 and Tie2. Tie2 was cloned in 1993 (Ziegler et al., (1993) *Oncogene* 8: 663-670) and is also known to those of skill in the art as "Tek." The vascular endothelial growth factor receptor kinases (VEGFRs) 1-4 are  
5 also believed to play an early role in vascular development processes, directing the differentiation of mesodermal cells into endothelial cells and the proliferation and migration of endothelial cells to form primitive tubular vessels (Ferrara & Davis-Smyth, (1997) *Endocrine Rev.* 18: 4-25; Borgström et al., (1996) *Cancer Res.* 56: 4032-4039; Adamis et al., (1996) *Arch. Ophthalmol.*  
10 114: 66-71.). The Tie RTKs are involved in the later stages of modulating cell-cell and cell-matrix interactions required for vascular remodeling and maturation (Koblizek et al., (1998) *Curr. Biol.* 8: 529-532; Witzenbichler et al., (1998) *J. Biol. Chem.* 273: 18514-18521).

Receptor tyrosine kinases comprise an extracellular ligand-binding  
15 domain (Tie2 has extracellular Ig and EGF homology domains) and an intracellular kinase domain. Binding of extracellular ligand is believed to promote dimerization, leading to autophosphorylation and activation of the kinase domain (reviewed in Lemmon & Schlessinger, (1994) *Trends Biochem. Sci.* 19: 459-463.) Stringent regulation of the phosphorylation state and  
20 activity of the cytoplasmic Tie2 receptor tyrosine kinase domain (hereinafter "Tie2K") is crucial to normal vasculature development and maintenance. Tie2 activity is precisely regulated by the opposing actions of agonistic and antagonistic extracellular ligands (Davis et al., (1996) *Cell* 87: 1161-1169; Maisonpierre et al., (1997) *Science* 277: 55-60; Valenzuela et al., (1999) *Proc.*

*Natl. Acad. Sci. USA* 96: 1904-1909). Tie2 activation requires autophosphorylation in response to binding its agonists, Ang1 and Ang4, whereas inactivation occurs in response to Ang2 and Ang3. Tie2 mutations, which result in ligand-independent and enhanced autophosphorylation, cause hereditary venous malformations (Vikkula et al., (1996) *Cell* 87: 1181-1190; 5 Calvert et al., (1999) *Hum. Mol. Genet.* 8: 1279-1289). Conversely, transgenic mice that express a kinase-inactive form of Tie2 or Tie2 null mice die *in utero* due to defects in their microvasculature (Sato et al., (1995) *Nature (London)* 376: 70-74; Dumont et al., (1994) *Genes Dev.* 8: 1897-1909.). 10 Inactivation of Ang1 or overexpression of Ang2 produces similar defects (Maisonpierre et al., (1997) *Science* 277: 55-60; Suri et al., (1996) *Cell* 87, 1171-1180; Suri et al., (1998) *Science* 282: 468-471).

The broad clinical potential of antiangiogenic therapy is just now being realized. Inhibition of either vascular endothelial growth factor receptor 2 15 (VEGFR2) or Tie2 by small molecules, by antibodies generated against the extracellular domain or by gene therapy have all been shown to reduce tumor progression (Borgström et al., (1996) *Cancer Res.* 56: 4032-4039; Lin et al., (1998) *Proc. Natl. Acad. Sci. USA* 95: 8829-8834). Development in the area of therapeutic treatments for angiogenic and vasculogenic disorders in 20 humans has been impeded, however, by the lack of a detailed structural understanding of Tie2. Detailed structural knowledge of the three-dimensional structure of the kinase domain (Tie2K) of this receptor will enhance the design of potent and selective modulators as therapeutic agents. Moreover, an in-depth understanding of the structure of Tie2K can be applied

to homologous kinases and will enhance the understanding of the entire field of receptor tyrosine kinase research.

Polypeptides, including Tie2K, have a three-dimensional structure determined by the primary amino acid sequence and the environment  
5 surrounding the polypeptide. This three-dimensional structure establishes the polypeptide's activity, stability, binding affinity, binding specificity, and other biochemical attributes. Thus, as noted above, knowledge of a protein's three-dimensional structure can provide much guidance in designing agents that mimic, inhibit, or improve its biological activity in soluble or membrane bound  
10 forms.

The three-dimensional structure of a polypeptide can be determined in a number of ways. Many of the most precise methods employ X-ray crystallography (See, e.g., Van Holde, (1971) Physical Biochemistry, Prentice-Hall, N. J., 221-239). This technique relies on the ability of crystalline lattices  
15 to diffract X-rays or other forms of radiation. Diffraction experiments suitable for determining the three-dimensional structure of macromolecules typically require high-quality crystals. Unfortunately, such crystals have been unavailable for Tie2K as well as many other proteins of interest. Thus, high-quality diffracting crystals of Tie2K would assist the determination of its three-  
20 dimensional structure.

Various methods for preparing crystalline proteins and polypeptides are known in the art (See, e.g., McPherson, et al., (1989) Preparation and Analysis of Protein Crystals, Robert E. Krieger Publishing Company, Malabar, Florida; Weber, (1991) Advances in Protein Chemistry 41:1-36; U.S. Pat. No.

4,672,108; and U.S. Pat. No. 4,833,233). There are multiple approaches to crystallizing polypeptides and slight differences in protein sequence often require variations in crystallization conditions, especially when the crystals must be suitable for X-ray diffraction studies. Thus, in spite of significant  
5 research, many proteins remain uncrystallized.

In addition to providing structural information, crystalline polypeptides provide other advantages. For example, the crystallization process itself further purifies the polypeptide, and satisfies one of the classical criteria for homogeneity. In fact, crystallization frequently provides unparalleled  
10 purification quality, removing impurities that are not removed by other purification methods such as HPLC, dialysis, conventional column chromatography, etc. Moreover, crystalline polypeptides are often stable at ambient temperatures and free of protease contamination and other degradation associated with solution storage. Crystalline polypeptides can  
15 also be useful as pharmaceutical preparations. Finally, crystallization techniques in general are largely free of problems such as denaturation associated with other stabilization methods (e.g., lyophilization). Once crystallization has been accomplished, crystallographic data provides useful structural information that can assist the design of compounds that can serve  
20 as agonists or antagonists, as described herein below. In addition, the crystal structure provides information useful to map the receptor binding domain which could then be mimicked by a small non-peptide molecule which can serve as an antagonist or agonist.



In an effort to elucidate the mechanisms underlying kinase activation as well as direct efforts to producing drugs to alleviate disease states in humans, the crystal structure of such proteins is often sought to be determined. The crystal structures of several protein serine/threonine kinases have been reported: cyclic-AMP-dependent protein kinase (cAPK; Knighton et al., (1991) *Science* 253: 407-414); cyclin-dependent kinase 2 (CDK2; DeBondt et al., (1993) *Nature* 363: 595-602); mitogen-activated protein kinase (MAPK; Zhang et al., (1994) *Nature* 367: 704-711); and twitchin kinase (Hu et al., (1994) *Nature* 369: 581-584). However, the crystalline structures of only three receptor tyrosine kinases have been determined to date-- the unphosphorylated apo form of the tyrosine kinase domain of the insulin receptor (Hubbard et al., (1994) *Nature* 372:746-754) and the phosphorylated tyrosine kinase domain of the insulin receptor complexed with substrate and an ATP analog (Hubbard, (1997) *EMBO J.* 16: 5572-5581); the unphosphorylated tyrosine kinase domain of FGFR1 in apo form and complexed with inhibitor (Mohammadi et al., (1996) *Cell* 86: 577-587); and the phosphorylated apo form of VEGFR2 (McTigue et al., (1999) *Structure* 7: 319-330).

Despite these reports, the ability to obtain crystalline forms of the tyrosine kinase domains of non-insulin receptor tyrosine kinases; i.e., cytoplasmic tyrosine kinases and/or receptor tyrosine kinases that undergo ligand-mediated dimerization, has not been realized. A particularly illuminating example is the EGF receptor; researchers armed with the knowledge of how to obtain crystals of the tyrosine kinase domains of both the

insulin receptor and serine/threonine kinases have attempted to obtain crystals of the tyrosine kinase domain of EGF receptor without success. And until disclosure of the present invention presented herein below, a detailed three-dimensional crystal structure of Tie2K has not been solved.

5        Clearly, the solved crystal structure of Tie2K would be invaluable in the design of modulators of Tie2K-mediated activity. Evaluation of the data obtained from the recent genome sequencing efforts has made it clear that Tie2 shares significant sequence homology with several hundred other kinases. Further, Tie2 shares the same three-dimensional fold with these  
10 other kinases. Thus, in theory, it might be considered feasible to design modulators of Tie2 based exclusively on the sequence and three-dimensional fold of a different kinase. This method, however, would likely be unproductive and certainly hindered by a lack of subtle structural details of the various binding sites and pertinent residues of Tie2K that a solved crystal structure  
15 would provide.

      The solved Tie2K crystal structure would be of immeasurable value in Tie2 modulator design because the solved crystal structure would provide structural details and insights necessary to design a modulator of Tie2 that maximizes preferred requirements for any modulator, potency and specificity.  
20 By exploiting the structural details obtained from a Tie2 crystal structure, it would be possible to design a Tie2 modulator that, despite Tie2's similarity with numerous other kinases, exploits the unique structural features of Tie2. A Tie2 modulator developed using structure-assisted design would take advantage of heretofore unknown Tie2 structural considerations and thus be

much more effective than a modulator developed using homology-based design. Potential or existent homology models cannot provide the necessary degree of specificity.

What is needed, therefore, is a crystallized form of the cytoplasmic Tie2 receptor kinase domain, Tie2K. Acquisition of Tie2K crystals will permit the three-dimensional structure of the cytoplasmic Tie2 receptor kinase domain to be determined. Knowledge of the three-dimensional structure of this polypeptide will facilitate the design of modulators of Tie2 receptor kinase activity. Such modulators can lead to therapeutic compounds to treat a wide range of vasculogenesis and angiogenesis-related disease states.

#### Disclosure of the Invention

A composition comprising a cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide in monoclinic crystalline form is disclosed. Preferably, the crystalline form has a space group of  $P2_1$ . More preferably, the crystalline form has lattice constants of  $a = 66 \text{ \AA}$ ,  $b = 92 \text{ \AA}$ ,  $c = 70 \text{ \AA}$ ,  $\alpha = 90^\circ$ ,  $\beta = 108^\circ$ ,  $\gamma = 90^\circ$ . Even more preferably, the crystalline form has a resolution of  $2.2 \text{ \AA}$  or better.

A composition comprising a cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide in orthorhombic crystalline form is also disclosed. Preferably, the crystalline form has a space group of  $P2_12_12_1$ . More preferably, the crystalline form has lattice constants of  $a = 79 \text{ \AA}$ ,  $b = 92 \text{ \AA}$ ,  $c = 109 \text{ \AA}$ ,  $\alpha = 90^\circ$ ,  $\beta = 90^\circ$ ,  $\gamma = 90^\circ$ . Even more preferably, the crystalline form has a resolution of  $2.5 \text{ \AA}$  or better.

A composition comprising a cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide in orthorhombic crystalline form is also disclosed. Preferably, the crystalline form has a space group of  $P2_12_12_1$ . More preferably, the crystalline form has lattice constants of  $a = 52 \text{ \AA}$ ,  $b = 77 \text{ \AA}$ ,  $c =$   
5  $79 \text{ \AA}$ ,  $\alpha = 90^\circ$ ,  $\beta = 90^\circ$ ,  $\gamma = 90^\circ$ . Even more preferably, the crystalline form has a resolution of  $2.2 \text{ \AA}$  or better.

A composition comprising a cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide in orthorhombic crystalline form and having a space group of  $C222_1$  and lattice constants of  $a = 95 \text{ \AA}$ ,  $b = 114 \text{ \AA}$ ,  $c = 78 \text{ \AA}$ ,  $\alpha = 90^\circ$ ,  
10  $\beta = 90^\circ$ ,  $\gamma = 90^\circ$  is also disclosed. Preferably, the crystalline form has a resolution of  $2.1 \text{ \AA}$  or better.

A method for determining the three-dimensional structure of a crystallized substantially pure cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide to a resolution of  $2.2 \text{ \AA}$  or better is disclosed. The method  
15 comprises: (a) crystallizing the cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide; and (b) analyzing the cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide to determine the three-dimensional structure of the crystallized Tie2 receptor tyrosine kinase domain polypeptide.

A method of designing a modulator of a cytoplasmic Tie2 receptor  
20 tyrosine kinase domain polypeptide is also disclosed. The method comprises: (a) designing a potential modulator of the cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide that will form bonds with amino acids in a substrate binding site based upon the structure the cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide; (b) synthesizing the modulator; and (c)

determining whether the potential modulator modulates the activity of the cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide.

A method of designing a modulator of a cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide is also disclosed. The method comprises:

- 5 (a) obtaining monoclinic or orthorhombic crystals of a substantially pure cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide; (b) evaluating the three-dimensional structure of the crystallized cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide; and (c) synthesizing potential modulators based on the three-dimensional crystal structure of the crystallized
- 10 cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide.

A method of screening for a modulator of a cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide is also disclosed. The method comprises:

- (a) providing a library of test samples; (b) contacting a crystalline form of cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide with each test
- 15 sample; (c) detecting an interaction between a test sample and the crystalline form of cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide; (d) identifying a test sample that interacts with a substantially pure cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide; and (e) isolating a test sample that interacts with a substantially pure cytoplasmic Tie2 receptor
- 20 tyrosine kinase domain polypeptide.

Also disclosed is an isolated and substantially pure nucleic acid sequence, the nucleic acid sequence coding for a Y897/Y1048F/S1119A Tie2K mutant polypeptide. A substantially pure Y897/Y1048F/S1119A Tie2K mutant polypeptide is also disclosed.

Accordingly, it is an object of the present invention to provide a novel crystalline form of a Tie2K polypeptide. The object is achieved in whole or in part by the present invention. An object of the invention having been stated hereinabove, other objects will be evident as the description proceeds, when  
5 taken in connection with the accompanying Laboratory Examples and Figures as best described hereinbelow.

### Brief Description of the Drawings

Figure 1 is a computer-generated ribbon diagram depicting the overall  
10 fold of Tie2K. The  $\beta$ -strands are labeled  $\beta 1$ ,  $\beta 2$ ,  $\beta 3$ ,  $\beta 4$ ,  $\beta 5$ ,  $\beta 7$  and  $\beta 8$ . Alpha helices are labeled  $\alpha C$ ,  $\alpha D$ ,  $\alpha E$ ,  $\alpha F$ ,  $\alpha G$ ,  $\alpha H$  and  $\alpha I$ . The nucleotide binding loop is designated **NBL**, the activation loop is labeled **AL**, the kinase insert domain is labeled **KID** and the C-terminal tail is labeled **CTT**. The amino and carboxy-termini are denoted by **N** and **C**. Breaks in the chain occur between  
15  $\beta$ -strand  $\beta 3$  and  $\alpha$ -helix  $\alpha C$  and in the activation loop due to crystal disorder. The figure was prepared with the RIBBONS software program (Carson & Bugg, (1986) J. Mol. Graphics 4: 121-122). An additional helix found in some kinases and located between helices  $\alpha E$  and  $\alpha F$  is labeled  $\alpha EF$ , in accordance with the convention adopted by researchers in the field.

20 Figure 2A is a computer-generated ribbon diagram depicting the N-terminal domains of Tie2K and FGFR1 in which the  $\alpha$ -carbons of the  $\beta$ -sheets have been superimposed. The N-termini of each structure are labeled as **N<sub>F</sub>** for FGFR1 and **N<sub>T</sub>** for Tie2K. The C-termini overlap and are labeled as **CC**. Beta strands  $\beta 1$ ,  $\beta 2$ ,  $\beta 3$ ,  $\beta 4$  and  $\beta 5$  are labeled. Nucleotide binding loop **NBL**

is labeled. Helix  $\alpha C$  is also labeled. The dashed line indicates the position of the disordered loop connecting  $\beta 3$  and  $\alpha$ -helix  $\alpha C$  in Tie2K.

Figure 2B is a computer-generated ribbon diagram depicting the C-terminal domains of Tie2K and FGFR1 in which the  $\alpha$ -carbons of the  $\alpha$ -helices have been superimposed. The C-terminal tail of Tie2K is labeled **CTT** and the kinase insert domain for Tie2K is labeled **KID**. The C-terminal tail of FGFR1 is labeled **C<sub>F</sub>** and the C-terminal tail of Tie2K is labeled **C<sub>T</sub>**. The N termini are labeled **NN**. Alpha helices  $\alpha D$ ,  $\alpha E$ ,  $\alpha F$ ,  $\alpha G$ ,  $\alpha H$  and  $\alpha I$  are labeled. Figures 2A and 2B were prepared with the QUANTA<sup>TM</sup> software program (QUANTA<sup>TM</sup>, Release 4.0. California, San Diego, 1994). An additional helix found in some kinases and located between helices  $\alpha E$  and  $\alpha F$  is labeled  $\alpha EF$ , in accordance with the convention adopted by researchers in the field.

Figure 3A is a computer-generated image depicting the activation, nucleotide binding and catalytic loops of Tie2K. The nucleotide binding loop is labeled **NBL**, and  $\alpha$ -helix  $\alpha C$  is shown. The activation loop is designated **AL**. The lysine and glutamic acid residues that form a salt bridge, **K855** and **E872**, are shown. The aspartate and arginine of the catalytic HDRLAAR motif (SEQ ID NO: 12), **D964** and **R963**, are labeled in the figure. The aspartate and phenylalanine of the AspPheGly motif at the start of the activation loop, **F983** and **D982**, are also labeled. Loops disordered in the crystal structures are indicated by dashed lines.

Figure 3B is a computer-generated image depicting the activation, nucleotide binding and catalytic loops of activated IRK. The nucleotide binding loop is labeled **NBL**, and  $\alpha$ -helix  $\alpha C$  is also shown. The activation

loop is designated **AL**. Residues of IRK that correspond to the residues of Tie2K labeled in Figure 3A are shown in Figure 3B. Specifically, the lysine and glutamic acid residues that form a salt bridge, **K1030** and **E1047** are labeled. The aspartate and arginine of the catalytic HDRLAAR motif (SEQ ID NO: 12), **D1132** and **R1131**, are identified in the figure. The aspartate and phenylalanine of the AspPheGly motif at the start of the activation loop, **F1151** and **D1150**, are also labeled.

Figure 3C is a computer-generated image depicting the activation, nucleotide binding and catalytic loops of unphosphorylated FGFR1. The nucleotide binding loop is labeled **NBL**, and  $\alpha$ -helix  $\alpha$ C is also shown. The activation loop is designated **AL**. Residues of FGFR1 that correspond to the residues of Tie2K labeled in Figure 3A are shown in Figure 3C. Specifically, the lysine and glutamic acid residues that form a salt bridge, **K514** and **E531** are labeled. The aspartate and arginine of the catalytic HDRLAAR motif (SEQ ID NO: 12), **D623** and **R622**, are labeled in the figure. The aspartate and phenylalanine of the AspPheGly motif at the start of the activation loop, **F642** and **D641**, are also labeled. Figures 3A-3C were generated with the QUANTA™ software program.

Figure 4 is a computer-generated image of the Tie2K ATP binding site. The superposition of the N-terminal  $\beta$ -sheets of Tie2K and activated IRK is shown.  $C_{\alpha}$ 's of  $\beta$ 1-  $\beta$ 5 were used to superimpose the structures of Tie2K and activated IRK (Hubbard et al., PDB ID: 1IR3; Accession No. P06213; available online at <http://www.rcsb.org/pdb/> ). The nucleotide binding site of Tie2K is



labeled as **NBL**, and **ATP** is shown in a bound conformation. Figure 4 was prepared with the QUANTA™ software program.

Figure 5 is a computer-generated image depicting the kinase insert domain and C-terminal tail of Tie2K. A ribbon diagram of the KIDs of Tie2K and IRK in which the  $\alpha$ -carbons of the C-terminal domain  $\alpha$ -helices have been superimposed is shown.  $\alpha$ -helices  $\alpha$ D,  $\alpha$ E,  $\alpha$ F and  $\alpha$ H are labeled in the figure. The KID and C-terminal tail for Tie2K are labeled as **KID<sub>T</sub>** and **CTT**, respectively. The KID for IRK is labeled **KID<sub>I</sub>**. Tyrosine 1101 (**Y1101**) and tyrosine 1112 (**Y1112**) of Tie2K are labeled. Figure 5 was prepared with the QUANTA™ software program.

Figure 6 is a computer-generated image depicting a noncrystallographic Tie2K dimer. The backbones of the two Tie2K polypeptides in the asymmetric unit are shown. The activation loops for the two Tie2K polypeptides are labeled **AL**. The nucleotide binding loops for the two Tie2K polypeptides are labeled **NBL**. The active site is labeled **AS**. A crystal contact is conserved at the noncrystallographic two-fold axis, and primarily involves the  $\beta$ 1 structural elements. The noncrystallographic two-fold axis and the dimer interface are indicated by an extended horizontal arrow. The crystal contact occurs at the interface of the two Tie2K structures and is centered around the labeled  $\beta$ 1 structures. Figure 6 was prepared with the QUANTA™ software program.

## Detailed Description of the Invention

I. Definitions

Following long-standing patent law convention, the terms "a" and "an"  
5 mean "one or more" when used in this application, including the claims.

As used herein, the term "Tie2K" means the kinase domain of the Tie2  
protein. In the context of mutant generation and analysis, the term is intended  
to include mutants having a mutation in the Tie2K domain, which is a  
component of the entire Tie2 protein. Thus, in the context of mutants, the  
10 term "Tie2K" is intended to include Tie2 proteins with a mutation in the Tie2K  
domain.

As used herein, the term "angiogenesis" means the generation of new  
blood vessels into a tissue or organ. Under normal physiological conditions,  
humans or animals undergo angiogenesis only in very specific restricted  
15 situations. For example, angiogenesis is normally observed in wound  
healing, fetal and embryonal development and formation of the corpus luteum,  
endometrium and placenta.

As used herein, the term "endothelium" means a thin layer of flat  
epithelial cells that lines serous cavities, lymph vessels, and blood vessels.

20 As used herein, the term "endothelial modulating activity" means the  
capability of a molecule to modulate angiogenesis in general and, for  
example, to stimulate or inhibit the growth of endothelial cells in culture.

As used herein, the term "mutation" carries its traditional connotation  
and means a change, inherited, naturally occurring or introduced, in a nucleic  
25 acid or polypeptide sequence, and is used in its sense as generally known to

those of skill in the art.

As used herein, the term "labeled" means the attachment of a moiety, capable of detection by spectroscopic, radiologic or other methods, to a probe molecule.

5       As used herein, the term "target cell" refers to a cell, into which it is desired to insert a nucleic acid sequence or polypeptide, or to otherwise effect a modification from conditions known to be standard in the unmodified cell. A nucleic acid sequence introduced into a target cell can be of variable length. Additionally, a nucleic acid sequence can enter a target cell as a component  
10 of a plasmid or other vector or as a naked sequence.

As used herein, the term "transcription" means a cellular process involving the interaction of an RNA polymerase with a gene that directs the expression as RNA of the structural information present in the coding sequences of the gene. The process includes, but is not limited to, the  
15 following steps: (a) the transcription initiation, (b) transcript elongation, (c) transcript splicing, (d) transcript capping, (e) transcript termination, (f) transcript polyadenylation, (g) nuclear export of the transcript, (h) transcript editing, and (i) stabilizing the transcript.

As used herein, the term "expression" generally refers to the cellular  
20 processes by which a biologically active polypeptide is produced from RNA.

As used herein, the term "transcription factor" means a cytoplasmic or nuclear protein which binds to such gene, or binds to an RNA transcript of such gene, or binds to another protein which binds to such gene or such RNA transcript or another protein which in turn binds to such gene or such RNA

transcript, so as to thereby modulate expression of the gene. Such modulation can additionally be achieved by other mechanisms; the essence of "transcription factor for a gene" is that the level of transcription of the gene is altered in some way.

5           As used herein, the term "hybridization" means the binding of a probe molecule, a molecule to which a detectable moiety has been bound, to a target sample.

          As used herein, the term "detecting" means confirming the presence of a target entity by observing the occurrence of a detectable signal, such as a  
10       radiologic or spectroscopic signal that will appear exclusively in the presence of the target entity.

          As used herein, the term "sequencing" means determining the ordered linear sequence of nucleic acids or amino acids of a DNA or protein target sample, using conventional manual or automated laboratory techniques.

15           As used herein, the term "isolated" means oligonucleotides substantially free of other nucleic acids, proteins, lipids, carbohydrates or other materials with which they can be associated, such association being either in cellular material or in a synthesis medium. The term can also be applied to polypeptides, in which case the polypeptide will be substantially  
20       free of nucleic acids, carbohydrates, lipids and other undesired polypeptides.

          As used herein, the term "substantially pure" means that the polynucleotide or polypeptide is substantially free of the sequences and molecules with which it is associated in its natural state, and those molecules used in the isolation procedure. The term "substantially free" means that the

sample is at least 50%, preferably at least 70%, more preferably 80% and most preferably 90% free of the materials and compounds with which it is associated in nature.

As used herein, the term "primer" means a sequence comprising two or  
5 more deoxyribonucleotides or ribonucleotides, preferably more than three, and more preferably more than eight and most preferably at least about 20 nucleotides of an exonic or intronic region. Such oligonucleotides are preferably between ten and thirty bases in length.

As used herein, the term "DNA segment" means a DNA molecule that  
10 has been isolated free of total genomic DNA of a particular species. For example, a DNA segment encoding a Tie2 or Tie2K polypeptide refers to a DNA segment that contains SEQ ID NO: 1, SEQ ID NO: 3 or SEQ ID NO: 5, yet is isolated away from, or purified free from, total genomic DNA of a source species, such as *Homo sapiens*. Included within the term "DNA segment" are  
15 DNA segments and smaller fragments of such segments, and also recombinant vectors, including, for example, plasmids, cosmids, phages, viruses, and the like.

As used herein, the phrase "enhancer-promoter" means a composite unit that contains both enhancer and promoter elements. An enhancer-  
20 promoter is operatively linked to a coding sequence that encodes at least one gene product.

As used herein, the phrase "operatively linked" means that an enhancer-promoter is connected to a coding sequence in such a way that the transcription of that coding sequence is controlled and regulated by that

enhancer-promoter. Techniques for operatively linking an enhancer-promoter to a coding sequence are well known in the art; the precise orientation and location relative to a coding sequence of interest is dependent, *inter alia*, upon the specific nature of the enhancer-promoter.

5           As used herein, the term "candidate substance" means a substance that is believed to interact with another moiety, for example a given ligand that is believed to interact with a complete Tie2 or Tie2K polypeptide, or fragment thereof, and which can be subsequently evaluated for such an interaction. Representative candidate compounds or substrates include xenobiotics such  
10 as drugs and other therapeutic agents, carcinogens and environmental pollutants, natural products and extracts, as well as endobiotics such as steroids, fatty acids and prostaglandins. Other examples of candidate substances that can be investigated using the methods of the present invention include, but are not restricted to, agonists and antagonists of a Tie2  
15 or Tie2K polypeptide, toxins and venoms, viral epitopes, hormones (e.g., opioid peptides, steroids, etc.), hormone receptors, peptides, enzymes, enzyme substrates, co-factors, lectins, sugars, oligonucleotides or nucleic acids, oligosaccharides, proteins, small molecules and monoclonal antibodies.

          As used herein, the term "biological activity" means any observable  
20 effect flowing from interaction between a Tie2 or Tie2K polypeptide and a ligand. Representative, but non-limiting, examples of biological activity in the context of the present invention include Tie2 autophosphorylation, dimerization of Tie2, angiogenesis, and vasculogenesis.

          As used herein, the term "modified" means an alteration from an

entity's normally occurring state. An entity can be modified by removing discrete chemical units or by adding discrete chemical units. The term "modified" encompasses detectable labels as well as those entities added as aids in purification.

5       As used herein, the terms "structure coordinates" and "structural coordinates" are interchangeable and mean mathematical coordinates derived from mathematical equations related to the patterns obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of a Tie2K molecule in crystal form. The diffraction data are used to calculate an electron  
10   density map of the repeating unit of the crystal. The electron density maps are used to establish the positions of the individual atoms within the unit cell of the crystal.

Those of skill in the art understand that a set of structure coordinates determined by X-ray crystallography is not without standard error. For the  
15   purpose of this invention, any set of structure coordinates for Tie2K or a Tie2K mutant that have a root mean square (RMS) deviation from ideal of no more than 1 Å, when superimposed using the polypeptide backbone atoms on the structure coordinates listed in Tables 2-5, shall be considered identical.

As used herein, the term "asymmetric unit" means part of a symmetric  
20   object from which the whole is built up by repeats. Thus, it is the smallest unit from which the object can be generated by the symmetry operations of its point group.

As used herein, the term "molecular replacement" means a method that involves generating a preliminary model of Tie2K or Tie2K mutant crystal

whose structure coordinates are unknown, by orienting and positioning a molecule whose structure coordinates are known (e.g., FGFR1 coordinates from Tables 6-10) within the unit cell of the unknown crystal so as best to account for the observed diffraction pattern of the unknown crystal. Phases  
5 can then be calculated from this model and combined with the observed amplitudes to give an approximate Fourier synthesis of the structure whose coordinates are unknown. This, in turn, can be subject to any of the several forms of refinement to provide a final, accurate structure of the unknown crystal (Lattman, (1985) in *Methods in Enzymology*, 115: 55-77). Using the  
10 structure coordinates of Tie2K provided by this invention, molecular replacement can be used to determine the structure coordinates of a crystalline mutant or homologue of Tie2K or of a different crystal form of Tie2K.

As used herein, the terms " $\beta$ -sheet" and "beta sheet" are  
15 interchangeable and mean the conformation of a polypeptide chain stretched into an extended zig-zig conformation. Portions of polypeptide chains that run "parallel" all run in the same direction. Polypeptide chains that are "antiparallel" run in the opposite direction from the parallel chains.

As used herein, the terms " $\alpha$ -helix" and "alpha helix" are  
20 interchangeable and mean the conformation of a polypeptide chain wherein the polypeptide backbone is wound around the long axis of the molecule in a left-handed or right-handed direction. The R groups of the amino acids protrude outward from the helical backbone, wherein the repeating unit of the



structure is a single turn of the helix, which extends about 0.56 nm along the long axis.

As used herein, the term "mutant" means a polypeptide which is obtained by replacing at least one amino acid residue in a native Tie2 or Tie2K polypeptide with a different amino acid residue and/or by adding and/or deleting amino acid residues within the native polypeptide or at the N- and/or C-terminus of a polypeptide corresponding to a native Tie2 or Tie2K and which has substantially the same three-dimensional structure as the native Tie2 or Tie2K from which it is derived. By having substantially the same three-dimensional structure is meant having a set of atomic structure coordinates that have a root mean square deviation (RMS deviation) of less than or equal to about 1Å when superimposed with the atomic structure coordinates of the native Tie2 or Tie2K from which the mutant is derived when at least about 50% to 100% of the C $\alpha$  atoms of the native Tie2 or Tie2K are included in the superposition. A mutant can have, but need not have, autophosphorylation activity.

As used herein, the term "space group" means a group or array of operations consistent with an infinitely extended regularly repeating pattern. It is the symmetry of a three-dimensional structure, or the arrangement of symmetry elements of a crystal. There are 230 space group symmetries possible; however, there are only 65 space group symmetries available for biological structures.

As used herein, the term "symmetry" means some spatial manipulation of an object resulting in an indistinguishable object. A symmetric object can, therefore, be superimposed on itself by some operation.

As used herein, the term "unit cell" means the fundamental portion of a crystal structure that is repeated infinitely by translation in three dimensions. A unit cell is characterized by three vectors  $a$ ,  $b$ , and  $c$ , not located in one plane, which form the edges of a parallelepiped. Angles  $\alpha$ ,  $\beta$  and  $\gamma$  define the angles between the vectors: angle  $\alpha$  is the angle between vectors  $b$  and  $c$ ; angle  $\beta$  is the angle between vectors  $a$  and  $c$ ; and angle  $\gamma$  is the angle between vectors  $a$  and  $b$ . The entire volume of a crystal can be constructed by regular assembly of unit cells; each unit cell comprises a complete representation of the unit of pattern, the repetition of which builds up the crystal.

As used herein, "monoclinic unit cell" means a unit cell wherein  $a \neq b \neq c$  and  $\alpha = \gamma = 90^\circ$  and  $\beta \neq 90^\circ$ . The vectors  $a$ ,  $b$  and  $c$  describe the unit cell edges and the angles  $\alpha$ ,  $\beta$ , and  $\gamma$  describe the unit cell angles.

As used herein, "orthorhombic unit cell" means a unit cell wherein  $a \neq b \neq c$ ; and  $\alpha = \beta = \gamma = 90^\circ$ . The vectors  $a$ ,  $b$  and  $c$  describe the unit cell edges and the angles  $\alpha$ ,  $\beta$ , and  $\gamma$  describe the unit cell angles.

As used herein, the term "crystal lattice" means the array of points defined by the vertices of packed unit cells.

As used herein, the term "active site" means that site in the Tie2K domain where substrate peptide binding, ATP binding and catalysis occur.

For Tie2, the active site comprises at least the activation loop and the nucleotide binding loop.

As used herein, the term "activation loop" refers to a loop in tyrosine kinase domains between the conserved AspPheGly sequence (residues 982-  
5 984 in Tie2K) and the conserved AlaProGlu sequence (residues 1006-1008 in Tie2K) that is believed to act as a regulatory loop.

As used herein, the terms "nucleotide-binding loop" and "glycine-rich loop" are synonymous and mean a loop in an RTK which contains the protein kinase-conserved glycine-rich consensus sequence. In Tie2K, this region  
10 corresponds to residues 831-836.

As used herein, the term "autophosphorylation site" means a residue or residues in Tie2K that is phosphorylated by a domain of Tie2 itself.

As used herein, the term "juxtamembrane region" means that portion of Tie2K located between the transmembrane helix and the tyrosine kinase  
15 domain, specifically, the first 35 cytoplasmic residues of Tie2K.

As used herein, the terms "kinase insert" and "kinase insert domain" are synonymous and mean an additional domain not found in non-receptor tyrosine kinases or serine/threonine kinases. It is found between helices  $\alpha$ D and  $\alpha$ E in the C-terminal domain of receptor tyrosine kinases and can vary  
20 greatly in sequence and length. In Tie2K, the kinase insert domain (KID) is positioned between helices  $\alpha$ D and  $\alpha$ E in the C-terminal domain (residues 916-936).

As used herein, the term "C-terminal tail" means that region of an RTK that extends beyond the final helix of the C-terminal domain of the RTK. In

Tie2K, the C-terminal region corresponds in sequence to amino acid residues 1099-1124. The C-terminal tail is known to interact with the SH2 domains of Grb2, Grb7, Grb14, Shp2 and other proteins.

As used herein, the term "N-terminal domain" means that region of an RTK that has a defined structure and precedes in sequence the KID. In Tie2K the N-terminal domain corresponds in sequence to amino acid residues 808-904 and comprises a twisted  $\beta$ -sheet and containing only a single  $\alpha$ -helix.

As used herein, the term "accessory proteins" means proteins that interact with Tie2 and modulate its activity. Interactions between Tie2 and its accessory proteins can be through hydrophobic interactions, hydrogen bonds, salt bridges or recognition of specific sequences or residues. For example, accessory proteins interact with Tie2 by binding specific phosphorylated tyrosine residues in the C-terminal tail of Tie2.

As used herein, the term "modulate" means an increase, decrease, or other alteration of any or all chemical and biological activities or properties of a wild-type or mutant Tie2 or Tie2K polypeptide.

## II. Description of Tables

Table 1 is a table summarizing the crystal and data statistics obtained from all four Tie2K crystal forms. Data on each of the unit cells is presented, including data on the crystal space group, unit cell dimensions, molecules per asymmetric cell and crystal resolution.

Table 2 is a table the atomic structure coordinate data obtained from X-ray diffraction from Tie2K crystal form I.

Table 3 is a table the atomic structure coordinate data obtained from X-ray diffraction from Tie2K crystal form II.

Table 4 is a table the atomic structure coordinate data obtained from X-ray diffraction from Tie2K crystal form III.

5        Table 5 is a table the atomic structure coordinate data obtained from X-ray diffraction from Tie2K crystal form IV.

Tables 6-10 are tables of the atomic structure coordinate data obtained from X-ray diffraction from an FGFR1 crystal (Mohammadi et al., PDB ID: 1FGK; Accession No. P11362; available online at <http://www.rcsb.org/pdb/> ).

10      The coordinate data from FGFR1 residues 464-485, 491-500, 506-578, 592-647 and 651-761 were used in the molecular replacement solution of crystal forms I-IV.

Table 6 is a table of the atomic coordinates for residues 464-485 (SEQ ID NO: 7) of FGFR1.

15        Table 7 is a table of the atomic coordinates for residues 491-500 (SEQ ID NO: 8) of FGFR1.

Table 8 is a table of the atomic coordinates for residues 506-578 (SEQ ID NO: 9) of FGFR1.

20      Table 9 is a table of the atomic coordinates for residues 592-647 (SEQ ID NO: 10) of FGFR1.

Table 10 is a table of the atomic coordinates for residues 651-761 (SEQ ID NO: 11) of FGFR1.

### III. Formation, Characterization and Solution of Generated Tie2K Crystals

#### III.A. Preparation of the Cytoplasmic Kinase Domain of A Tie2

##### Polypeptide

Tie2K, comprising residues 808-1124 of Tie2, was expressed in  
5 baculovirus-infected Sf9 insect cells. The first 35 cytoplasmic residues, which  
are juxtaposed against the membrane, were not included in the construct. A  
hexahistidine tag was added at the N-terminus of the polypeptide to aid in the  
polypeptide purification process. Baculovirus-expressed Tie2K was  
heterogeneous with respect to phosphorylation. Preparations contained a  
10 mixture of proteins with zero to six phosphoryl groups that could not be fully  
separated by standard chromatographic procedures.

#### III.B. Crystal Forms of the Cytoplasmic Kinase Domain of Tie2

##### Polypeptide

15 Crystallization screens were initially performed using a mixture of the  
non-, mono- and diphosphorylated species. Three different crystal forms of  
Tie2K were obtained. As shown in Table 1, crystal forms I and II contained  
unphosphorylated protein, while crystal form III contained mono-  
phosphorylated protein. A mutant form of Tie2K, discussed below, provided a  
20 fourth crystal form.

#### III.C. Mapping of Phosphorylation Sites by Mass Spectrometry

Three (two major and one minor) phosphorylation sites were mapped  
by mass spectrometry.

### III.D. Mutation of Phosphorylation Sites

The two major sites, tyrosine 897 and serine 1119, were mutated to phenylalanine and alanine respectively, while the minor site, tyrosine 1048, was mutated to phenylalanine. The mutant form of Tie2K was purified to  
5 homogeneity as unphosphorylated protein and gave rise to crystal form IV, coordinate data for which is presented in Table 5.

### III.E. Solving the Three-Dimensional Structure of Tie2K by Molecular Replacement

10 The structure of crystal form I was solved by molecular replacement using the structure of the unphosphorylated kinase domain of FGFR1 (Mohammadi et al., (1996) *Cell* 86: 577-87) as a search model. The structure was refined to an R-factor of 19% to a resolution of about 2.2 Å. Six residues at the N-terminus, three residues at the C-terminus, four residues in the  
15 activation loop, and six residues connecting  $\beta 3$  and  $\alpha C$  were disordered and could not be modeled. The structures of crystal forms II, III and IV were solved by molecular replacement using the structure determined for crystal form I. The Tie2K structure in all four crystal forms was essentially identical, suggesting that conformations observed in the structure are not due to crystal  
20 packing forces. Residues disordered in crystal form I were also disordered in crystal forms II, III and IV. Superposition of all backbone  $\alpha$ -carbons yielded a root mean square deviation (RMSD) of 0.18 Å for form I versus form II, 0.47 Å for form I versus form III, and 0.45 Å for form I versus form IV.

### III.F. The Three-Dimensional Structure of the Cytoplasmic Tie2 Receptor Kinase Domain

The present invention discloses four crystalline forms of the Tie2K.  
5 Using these four crystalline forms, the three-dimensional structure of Tie2K  
was solved to a resolution of about 2.2 Å. Crystal form I was solved using  
molecular replacement techniques. The solved structure of crystal form I was  
then used as a template for the solution of crystal forms II, III and IV using  
molecular replacement methodology. Crystal forms I and II comprise  
10 unphosphorylated protein. Crystal form III comprises monophosphorylated  
protein. Crystal form IV comprises unphosphorylated protein. A summary of  
the crystal data for all four crystal forms is presented in Table 1, and  
coordinate data for crystal forms I-IV are presented in Tables 2-5,  
respectively.

15

#### III.F.1. Overview of the Three-Dimensional Structure of Tie2K

A ribbon diagram of the C<sub>α</sub> backbone of Tie2K is depicted in Figure 1.  
The kinase secondary structural elements are labeled according to the  
convention adopted by researchers in the field and originally given for cAPK  
20 (Knighton et al., (1991) Science 253: 407-413.). Tie2K folds into two  
domains, with catalysis occurring in a cleft between the two domains. As  
depicted in Figure 1, residues in the N-terminal domain **N** are primarily  
responsible for ligating ATP, while residues in the C-terminal domain **C** are  
involved in catalysis and substrate binding.



Continuing with Figure 1, the N-terminal domain of Tie2K (residues 808-904) folds into a twisted  $\beta$ -sheet and one  $\alpha$ -helix. The larger C-terminal domain (residues 905-1124) contains seven  $\alpha$ -helices, helices  $\alpha$ D through  $\alpha$ I, and two anti-parallel  $\beta$ -strands,  $\beta$ 7 and  $\beta$ 8. These two strands are positioned at the interdomain interface adjacent to the N-terminal  $\beta$ -sheet. Kinase insert domain **KID** comprises 2 short helical segments that pack against the C-terminal lobe and the extended C-terminal tail. Like other kinases, Tie2K also contains functionally important loop regions: the glycine-rich nucleotide binding loop **NBL** (residues 831-836), the catalytic loop **CL** (residues 962-968) and the activation loop **AL** (residues 982-1008).

### III.F.2. Comparison of the Structure of Tie2K to the Structure of FGFR1

Of the reported kinase structures, the overall structure of Tie2K most closely resembles the catalytic domain of fibroblast growth factor receptor 1 (FGFR1, Mohammadi et al., (1996) *Cell* 86: 577-87), with which it shares ~45% sequence identity. Superposition of the 5  $\beta$ -strands in the N-terminal domains of Tie2K and FGFR1 yielded an N-terminal domain  $C_\alpha$  RMSD of 0.76 Å; superposition of the C-terminal domains using  $\alpha$ -carbons from the 7  $\alpha$ -helices gave a C-terminal domain  $C_\alpha$  RMSD of 0.58 Å. Like unphosphorylated FGFR1, Tie2K is in an opened conformation with a relative rotation of approximately 15° between the N- and C-terminal lobes when compared to the closed, active structure of insulin receptor kinase (IRK)

(Hubbard, (1997) *EMBO J.* 16: 5572-5581), an RTK predicted to have similar structure.

The beta sheet topologies in the N-terminal domain of FGFR1 and Tie2K are quite similar, as depicted in Figure 2A. Significant differences are observed, however, in three distinct regions: the nucleotide binding loop **NBL**, the loops connecting  $\beta 3$ - $\alpha C$  and  $\beta 4$ - $\beta 5$ , and the position of the C-helix. Compared with FGFR1,  $\beta$  strands  $\beta 3$ ,  $\beta 4$  and  $\beta 5$  of Tie2K contain one additional residue. This difference produces a change in the conformation of the loop regions connecting these sheets. The extension of the  $\beta 3$ - $\beta 4$ - $\beta 5$  sheet displaces residues in the C-helix of Tie2K by 2.5 to 5.5 Å from their equivalent positions in FGFR1. Additionally, six Tie2K residues in the loop connecting  $\beta 3$  with  $\alpha C$ , residues alanine 861 (A861) through histidine 866 (H866), are disordered in all four crystal forms. Therefore, only 3.5 turns of the C-helix are observed for Tie2K, as opposed to 5 turns observed in FGFR1.

In the N-terminal domain of a number of kinases, two conserved, charged residues form a salt bridge in order to correctly position the  $\alpha$  and  $\beta$  phosphates of ATP for catalysis. In Tie2K these residues correspond to lysine 855 (K855) on  $\beta 3$  and glutamate 872 (E872) on helix  $\alpha C$ . Due to the shift in helix  $\alpha C$ , these residues are about 7.2 Å apart compared with the approximately 3-4 Å distance observed in other kinase structures (Hubbard et al., (1994) *Nature* 372: 746-754; Hubbard, (1997) *EMBO J.* 16: 5572-5581; Mohammadi et al., (1996) *Cell* 86: 577-87; McTigue et al., (1999) *Structure* 7: 319-330). While the shift in helix  $\alpha C$  is not as dramatic as the shift observed in the structures of inactive cdk2 as compared to the activated cdk2/cyclinA

complex, which known to be 8.5 Å (Jeffrey et al., (1995) *Nature* 376: 313-320), the conformational change required to bring these residues into proper alignment for ATP binding is not obvious.

Figure 2B demonstrates that the C-terminal lobes of Tie2K and FGFR1  
5 are also quite similar in structure and position, except for the positions of the activation loop **AL** and kinase insert domain **KID**, which is disordered in FGFR1. The C-terminal tail was included in the Tie2K construct but not in FGFR1, IRK and VEGFR2; and is observed in the Tie2K crystal structure. Continuing with Figure 2B, the C-terminal tail has an extended conformation  
10 that packs under the **KID**, runs along helices  $\alpha$ I,  $\alpha$ F and  $\alpha$ E, and ends near the substrate binding site.

### III.F.3. The Activation Loop and Catalytic Residues

Protein kinases contain a large flexible loop, called the activation loop,  
15 or A-loop, whose conformation is believed to regulate kinase activity. In many kinases, the conformation of the A-loop is controlled by the phosphorylation of specific residues within the A-loop. Johnson et al., (1996) *Cell* 85: 149-158. The activation loop generally begins with a conserved AspPheGly sequence, identified in Tie2K as residues 982-984, and ends at a conserved AlaProGlu,  
20 identified in Tie2K as residues 1006-1008. Johnson et al., (1996) *Cell* 85: 149-158. In structures of inactive kinases, this loop often blocks either the substrate or ATP binding sites. Hubbard et al., (1994) *Nature* 372: 746-754; Mohammadi et al., (1996) *Cell* 86: 577-87; McTigue et al., (1999) *Structure* 7: 319-330. Upon phosphorylation, the A-loop is repositioned to contact

residues in the C-terminal domain. Hubbard (1997) *EMBO J.* 16: 5572-5581.

The activating phosphate can then interact with a cluster of basic residues, which includes a conserved arginine (corresponding to arginine 963, R963, in Tie2K) that precedes a catalytic aspartate residue (aspartate 964, D964, in Tie2K). The aspartyl residue of the AspPheGly motif ligates a  $Mg^{2+}$  ion, which in turn contacts the  $\beta$  and  $\gamma$  phosphates of ATP.

The activation loop of Tie2K corresponds to residues 982-1008 and contains a single tyrosine at position 992. The conserved AlaProGlu sequence of protein kinases occurs as AlalleGlu in Tie2. In the Tie2K structure of the present invention, the A-loop more closely resembles that of activated IRK than that seen for inactive, unphosphorylated FGFR1, as is depicted in Figure 3A, 3B and 3C.

Continuing with Figures 3A-3C, four residues near the N-terminal end of Tie2K's A-loop **AL**, residues threonine 996 (**T996**) through arginine 999 (**R999**), are disordered. All attempts to phosphorylate **Y992** (which is found in A-loop **AL**) using purified wild-type protein have been unsuccessful. However, when tyrosines 897 and 1048 and serine 1119 were mutated to phenylalanine and alanine respectively, the purified protein could be quantitatively phosphorylated on **Y992**. While it is not the applicants' desire to be bound to any theory, it is postulated that these observations suggest that the mode by which Tie2 is activated is complex and could differ from that found in other RTKs (Johnson et al., (1996) *Cell* 85, 149-158).

The conformation of the conserved AspPheGly motif of the Tie2K activation loop is also significantly different than that seen in other kinase

structures (Hubbard et al., (1994) *Nature* 372: 746-754; Hubbard (1997) *EMBO J.* 16: 5572-5581; Mohammadi et al., (1996) *Cell* 86: 577-87; McTigue et al., (1999) *Structure* 7: 319-330). The side chains of **D982** and **F983** point in directions opposite to those observed in nonphosphorylated FGFR1 and  
5 activated IRK (Figures 3A, 3B and 3C). As seen in Figures 3A-3C, the aspartate 982 (**D982**) side chain is directed towards the back of the pocket, away from the ATP binding site. The Tie2K side chain of phenylalanine 983 (**F983**) extends towards solvent and is sandwiched between the side chains of **K855** of  $\beta 3$  and **E872** of helix  $\alpha C$ , the conserved residues which form the salt  
10 bridge required to correctly position the phosphates of ATP. Although the Tie2K activation loop adopts an "active-like" conformation overall, the AspPheGly motif at the beginning of this loop has a conformation which could potentially inhibit ATP binding.

The catalytic loop of protein kinases lies between helices  $\alpha E$  and  $\beta 7$   
15 and contains an invariant aspartic acid (**D964** in Tie2K) that serves as the catalytic base in the phosphotransfer reaction (Johnson et al., (1996) *Cell* 85: 149-158). The catalytic loops of Tie2, FGFR1, VEGFR2 and IRK are identical in sequence, each containing the HRDLAARN (SEQ ID NO: 12) sequence. Hubbard et al., (1994) *Nature* 372: 746-754; Mohammadi et al., (1996) *Cell*  
20 86: 577-87; McTigue et al., (1999) *Structure* 7: 319-330. As depicted in Figures 3A-3C, the backbone and side chain positions of this loop in Tie2K are similar to those in the unliganded FGFR1 and VEGFR2 and in the ternary phosphorylated IRK complex structures.

#### III.F.4. The Nucleotide Binding Loop

The nucleotide binding loop of an RTK contains residues responsible for binding the triphosphate moiety of ATP in the correct position for catalysis (Johnson et al., (1996) *Cell* 85: 149-158). This glycine-rich loop is believed to  
5 be quite flexible and is often either disordered or has high *b*-factors (which are indicative of the degree of flexibility of a protein segment) in many unliganded kinase structures. Mohammadi et al., (1996) *Cell* 86: 577-87; McTigue et al., (1999) *Structure* 7: 319-330.

In Tie2K, this loop adopts a unique self-inhibitory conformation with  
10 residues 832-836 occupying the ATP binding site, exemplified in Figure 4. The  $\gamma$  carboxylate of glutamine 832 (**E832**), if protonated, could form a hydrogen bond with the backbone carbonyl of glutamine 903 (**E903**). The backbone carbonyl of E903 presumably participates in the binding of ATP through a hydrogen bond to the 6-amino group of the nucleotide. The  $\alpha$  and  $\beta$   
15 phosphate binding sites of ATP are occupied by asparagine 834 (**N834**) and glycine 836 (**G836**). Phenylalanine 835 (**F835**) sits in a pocket at the back of the site formed by the side chains of lysine 855 (**K855**), isoleucine 886 (**I886**), isoleucine 902 (**I902**) and phenylalanine 983 (**F983**). Asparagine 834 (**N834**) occupies the site of the conserved aspartate of the AspPheGly motif in the A-  
20 loop that binds  $Mg^{2+}$  and the  $\gamma$  phosphate of ATP.

ATP was modeled into the active site of Tie2K based on the structure of activated IRK. As depicted in Figure 4, the nucleotide binding loop **NBL** precludes the binding of ATP.

### III.F.5. The Kinase Insert Domain

Many RTKs contain a kinase insert domain (KID) of variable length and sequence between helices  $\alpha$ D and  $\alpha$ E in their C-terminal domain. This insert can be as short as 12 residues or as long as 97 residues, as in IRK and  
5 platelet derived growth factor receptor  $\beta$  (PDGFR $\beta$ ), respectively. Hubbard et al., (1994) *Nature* 372: 746-754; Heidaran (1991) *Mol. Cell. Biol.* 11: 134-142. Deletion or mutation of this insert in other kinases revealed that the KID is not necessary for intrinsic kinase activity. McTigue et al., (1999) *Structure* 7: 319-330; Heidaran et al., (1991) *Mol. Cell. Biol.* 11: 134-142; Taylor et al., (1989)  
10 *EMBO J.* 8: 2029-2037. However, this kinase insert domain might be important for protein-protein interactions involved in signal transduction via autophosphorylation of KID tyrosine residues. Heidaran et al., (1991) *Mol. Cell. Biol.* 11: 134-142; Taylor et al., (1989) *EMBO J.* 8: 2029-2037. In Tie2, this region corresponds to residues 916-936 and does not contain tyrosine  
15 residues.

Due to the lack of sequence conservation in this domain, structural conservation is also not expected. In FGFR1, the KID is apparently quite mobile and disordered in the crystal structure of the unliganded protein. (Mohammadi et al., *Cell* 86: 577-87) In VEGFR2, the KID was deleted in the  
20 construct used for structural studies (McTigue et al., (1999) *Structure* 7: 319-330). In the IRK structure, this region, comprising proline 1093 (P1093) to glycine 1110 (G1100), is proline-rich and forms a loop that folds towards the N-terminal domain (Hubbard et al., (1994) *Nature* 372: 746-754). In Tie2K, the KID comprises two short helical segments connected by a turn, as

depicted in Figure 5, and packs against residues 1104-1112 in the C-terminal tail.

### III.F.6. Interaction of the C-terminal Tail With Accessory Proteins

5       The C-terminal tail of Tie2 has been shown to bind a number of proteins containing src homology 2 (SH2) and phosphotyrosine binding (PTB) domains in a phosphotyrosine-dependent manner. Numerous reports suggest that tyrosines 1101 (Y1101) and 1112 (Y1112) (as shown in Figure 5) in the C-terminal tail interact with the SH2 domains of Grb2, Grb7, Grb14, 10 Shp2, the p85 subunit of PI3 kinase, and the PTB domain of Dok-R. Huang et al., (1995) *Oncogene* 11: 2097-2103; Jones & Dumont, (1998) *Oncogene* 17: 1097-1108; Kontos et al., (1998) *Mol. Cell. Biol.* 18: 4131-4140; Jones et al., (1999) *J. Biol. Chem.* 274: 30896-30905; Korpelainen et al., (1999) *Oncogene* 18: 1-8.

15       In the unliganded crystal structure of the present invention, the hydroxyls of tyrosine 1101 (Y1101) and tyrosine 1112 (Y1112) are not solvent exposed, and appear to play a structural role, as depicted in Figure 5. The hydroxyl of Y1101 hydrogen bonds to the side chain of E759 (not shown in Figure 5) while the phenyl ring is packed between the side chains of M757 20 and K762 (not shown in Figure 5). The hydroxyl of Y1112 hydrogen bonds to the main chain NH and carbonyl oxygen of L579 and A592 respectively. The phenyl ring of Y1112 sits in a hydrophobic pocket formed by the side chains of L696, L579, F1114, and R577 (not shown in Figure 5). Mass spectroscopic analysis of the baculovirus-expressed Tie2K showed that Y897 and Y1048,



which point directly out into solvent, are partially phosphorylated. But, there was no evidence for phosphorylation of Y1101 or Y1112.

In the unphosphorylated FGFR1 and IRK structures, the activation loop blocks access to the substrate binding site. Hubbard et al., (1994) *Nature* 372: 746-754; Mohammadi et al., (1996) *Cell* 86: 577-87. Continuing with Figure 5, in Tie2K the activation loop adopts an "active-like" conformation while the end of the C-terminal tail **CTT** could block access to the substrate binding site. The last ordered residue E1120 (not shown in Figure 5) of the C-terminal tail, **CTT**, is positioned where the substrate residue preceding the tyrosine would bind. While it is not the applicants' desire to be bound to any theory, it is postulated that in view of this data, the C-terminal tail undergoes a conformational change upon activation of the protein, exposing both the substrate binding site and Y1101 and Y1112 for phosphorylation and signaling.

15

### III.G. Mutational Analysis of Tie2K Crystal Forms

Two mutations in the N-terminal domain of Tie2, R849W and Y897S, have been identified in humans, and segregate with an autosomal dominant condition known as Vascular Dysmorphogenesis. Vikkula et al., (1996) *Cell* 87: 1181-1190; Calvert et al., (1999) *Hum. Mol. Genet.* 8: 1279-1289. This condition is characterized by lesions consisting of haphazardly-arranged, dilated blood vessels that lack or have a reduced smooth muscle layer and little to no supportive tissue. These two mutations result in ligand-independent hyperphosphorylation of Tie2. Vikkula et al., (1996) *Cell* 87:

20

1181-1190; Calvert et al., (1999) *Hum. Mol. Genet.* 8: 1279-1289. It has been suggested that they either relieve autoinhibition of the kinase or promote dimerization in the absence of ligand (Vikkula et al., (1996) *Cell* 87: 1181-1190).

- 5           The Tie2K crystal forms I and II of the present invention, which comprise unphosphorylated protein, have 2 molecules in the asymmetric unit. Crystal form III, comprising protein mono-phosphorylated at the tyrosine 897 position, contains only one molecule in the asymmetric unit. In the two unphosphorylated crystal forms, one crystal contact ( $\sim 1096 \text{ \AA}^2$ ) is conserved
- 10   at the noncrystallographic two-fold axis, depicted in Figure 6 as an extended horizontal arrow. This contact primarily involves  $\beta 1$  as well as residues from the ends of  $\beta 2$ ,  $\beta 3$  and  $\beta 4$  in the N-terminal domain. Both residues R849 and Y897 (not shown in Figure 6) sit at this crystal contact. Phenylalanine 826, valine 829 and leucine 839 form the hydrophobic core of this interface.
- 15   Tyrosine 897, tyrosine 899, arginine 849 and aspartic acid 828 are located at the edges of the interface. Arginine 849, the first residue of  $\beta 3$ , makes a weak hydrogen bond to glutamine 837 of the neighboring molecule. The side chain of R849 is packed between the side chains of Y897 and V829 from the neighboring molecule. Tyrosine 897 is located on the loop connecting  $\beta 4$  and
- 20    $\beta 5$  and packs against arginine 849. While it is not the applicants' desire to be bound to any theory, it is postulated that mutation of arginine 849 to tryptophan could allow for better packing at this predominantly hydrophobic interface.

Again, while it is not the applicants' desire to be bound to any theory, it is further postulated that phosphorylation of Y897 would be difficult to accommodate at this tight crystal contact and therefore would lead to crystal form III. If this extensive crystal contact is in fact a biologically significant dimer interface, the phosphorylation state of Y897 could be another mechanism of controlling the activity of Tie2. When Y897 is phosphorylated, the cytoplasmic kinase domains cannot dimerize; but when unphosphorylated or mutated to a serine, Tie2K dimerization would be favored. This is further supported by the observation that purified wild-type Tie2K, a significant fraction of which is phosphorylated on tyrosine 897, could not appreciably autophosphorylate tyrosine 992 in the activation loop. In contrast, the Y897F/Y1048F/S1119A mutant could autophosphorylate Y992, leading to an approximately 100-fold increase in kinase activity. Additionally, Tie2, when phosphorylated on Y897, has been shown to bind the protein tyrosine phosphatase Shp2, which can also play a role in down regulation of Tie2 activity. Huang et al., (1995) *Oncogene* 11: 2097-2103; Jones et al., (1999) *J. Biol. Chem.* 274: 30896-30905.

#### IV. Uses of Tie2K Crystals and the Three-Dimensional Structure of Tie2K

20

##### IV.A. Design and Development of Tie2K Modulators

The knowledge of the structure of the cytoplasmic Tie2 receptor tyrosine kinase domain, an aspect of the present invention, provides a tool for investigating the mechanism of action of the Tie2 and Tie2K polypeptides in a

subject. For example, various computer models, as described herein, can predict binding of various substrate molecules to Tie2K. Upon discovering that such binding takes place, knowledge of the protein structure then allows design and synthesis of small molecules that mimic the functional binding of  
5 the substrate to Tie2K. This is the method of "rational" drug design, further described herein.

Use of the isolated and purified Tie2K structure of the present invention in rational drug design is thus provided in accordance with the present invention. Rational drug design techniques are described in U.S. Patent Nos.  
10 5,834,228 and 5,872,011, incorporated herein in their entirety.

#### IV.A.1. Rational Drug Design

A method of identifying modulators of the activity of Tie2 or Tie2K using rational drug design is provided in accordance with the present invention. The  
15 method comprises the steps of designing a potential modulator for the Tie2 or Tie2K polypeptide of the present invention that will form non-covalent bonds with amino acids at a binding site based upon a crystalline form of the Tie2 or Tie2K polypeptide; synthesizing the modulator; and determining whether the potential modulator modulates the activity of the Tie2 or Tie2K polypeptide.  
20 Modulators can be synthesized using techniques known to those of ordinary skill in the art.

The determination of whether the modulator modulates the biological activity of the Tie2 or Tie2K polypeptide can be made in accordance with the screening methods disclosed herein, or by other screening methods known to

those of skill in the art. Preferably, the Tie2 polypeptide comprises the amino acid sequence of SEQ ID NO: 2, and the Tie2K polypeptide comprises the amino acid sequence of SEQ ID NO: 4. In another preferred embodiment, the Tie2K polypeptide comprises the amino acid sequence of SEQ ID NO: 6.

5

#### IV.A.2. Methods for Using the Tie2K Structural Coordinates For Molecular Design

For the first time, the present invention permits the use of molecular design techniques to design, select and synthesize chemical entities and compounds, including modulatory compounds, capable of binding to the active site or accessory binding site of Tie2 and Tie2K, in whole or in part.

In accordance with the present invention the structure coordinates of crystalline Tie2K can be used to design compounds that bind to the Tie2K domain and alter the properties of Tie2K, e.g., autophosphorylation ability, in different ways. For example, the present invention provides for the design of compounds that act as competitive inhibitors of the Tie2 enzyme by binding to all, or a portion of, the binding sites on the Tie2K domain. The present invention also provides for the design of compounds that can act as uncompetitive inhibitors of the Tie2K enzyme. These compounds can bind to all, or a portion of, an accessory binding site of a Tie2 that is already binding its substrate and can, therefore, be more potent and less non-specific than known competitive inhibitors that compete only for the Tie2K substrate or nucleotide binding site. Similarly, non-competitive inhibitors that bind to and inhibit Tie2K, whether or not it is bound to another chemical entity, can be designed using the Tie2K structure coordinates of this invention.

A second design approach is to probe a Tie2K crystal with molecules comprising a variety of different chemical entities to determine optimal sites for interaction between candidate Tie2K modulators and the polypeptide. For example, high resolution X-ray diffraction data collected from crystals saturated with solvent allows the determination of the site where each type of solvent molecule adheres. Small molecules that bind tightly to those sites can then be designed and synthesized and tested for their Tie2K modulator activity (Allen et al., (1996) *J. Phys. Chem.* 100(7): 2606-2611).

10      IV.A.3.      Methods of Designing Tie2K Modulator  
                         Compounds

The design of candidate substances, also referred to as "compounds" or "candidate compounds", that bind to or inhibit Tie2K according to the present invention generally involves consideration of two factors. First, the compound must be capable of physically and structurally associating with Tie2K. Non-covalent molecular interactions important in the association of Tie2K with its substrate include hydrogen bonding, van der Waals and hydrophobic interactions.

Second, the compound must be able to assume a conformation that allows it to associate with Tie2K. Although certain portions of the compound will not directly participate in this association with Tie2K, those portions can still influence the overall conformation of the molecule. This, in turn, can have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity

or compound in relation to all or a portion of the binding site, e.g., active site or accessory binding site of Tie2K, or the spacing between functional groups of a compound comprising several chemical entities that directly interact with Tie2K.

5           The potential modulatory or binding effect of a chemical compound on Tie2K can be analyzed prior to its actual synthesis and testing by the use of computer modeling techniques. If the theoretical structure of the given compound suggests insufficient interaction and association between it and Tie2K, synthesis and testing of the compound is obviated. However, if  
10 computer modeling indicates a strong interaction, the molecule can then be synthesized and tested for its ability to bind and inhibit Tie2K. In this manner, synthesis of unproductive or inoperative compounds can be avoided.

A modulatory or other binding compound of Tie2K can be computationally evaluated and designed by means of a series of steps in  
15 which chemical entities or fragments are screened and selected for their ability to associate with the individual binding sites or other areas of Tie2K.

One of ordinary skill in the art can use one of several methods to screen chemical entities or fragments for their ability to associate with Tie2K and, more particularly, with the individual binding sites of the Tie2K active site  
20 or an accessory binding site. This process can begin by visual inspection of, for example, the active site on a computer screen based on the Tie2K coordinates in Tables 2-5. Selected fragments or chemical entities can then be positioned in a variety of orientations, or docked, within an individual binding site of Tie2K as defined herein above. Docking can be accomplished

using software programs such as those available under the tradenames QUANTA™ and SYBYL™ (Tripos, Inc., St. Louis, Missouri), followed by energy minimization and molecular dynamics with standard molecular mechanics forcefields, such as CHARM and AMBER.

5       Specialized computer programs can also assist in the process of selecting fragments or chemical entities. These include:

1. GRID™ program, version 17 (Goodford, (1985) *J. Med. Chem.* 28: 849-857), which is available from Molecular Discovery Ltd., Oxford, UK;
2. MCSS™ program (Miranker & Karplus, (1991) *Proteins* 11: 29-34),  
10    which is available from Molecular Simulations, Inc., San Diego, California;
3. AUTODOCK™ 3.0 program (Goodsell & Olsen, (1990) *Proteins* 8: 195-202), which is available from the Scripps Research Institute, La Jolla, California; and
4. DOCK™ 4.0 program (Kuntz et al., (1992) *J. Mol. Biol.* 161: 269-  
15    288), which is available from the University of California, San Francisco, California.

Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound or modulator. Assembly can be proceed by visual inspection of the relationship of the fragments to each other  
20    on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of Tie2K. Manual model building using software such as QUANTA™ or SYBYL™ typically follows.

Useful programs to aid one of ordinary skill in the art in connecting the individual chemical entities or fragments include:



1. CAVEAT™ program (Bartlett et al., (1989) *Special Pub.*, *Royal Chem. Soc.* 78: 182-196), which is available from the University of California, Berkeley, California;

2. 3D Database systems, such as MACCS-3D™ system program,  
5 which is available from MDL Information Systems, San Leandro, California.

This area is reviewed in Martin, (1992) *J. Med. Chem.* 35: 2145-2154; and

3. HOOK™ program (Eisen et al., (1994). *Proteins*: 19: 199-221),  
which is available from Molecular Simulations, Inc., San Diego, California.

Instead of proceeding to build a Tie2K modulator in a step-wise fashion  
10 one fragment or chemical entity at a time as described above, modulatory or  
other Tie2K binding compounds can be designed as a whole or *de novo* using  
either an empty binding site or optionally including some portion(s) of a known  
modulator(s). Applicable methods can employ the following software  
programs:

15 1. LUDI™ program (Bohm, (1992) *J. Comp. Aid. Molec. Design*, 6: 61-  
78), which is available from Molecular Simulations, Inc., San Diego, California;

2. LEGEND™ program (Nishibata & Itai, (1991) *Tetrahedron* 47:  
8985); and

3. LEAPFROG™, which is available from Tripos Associates, St. Louis,  
20 Missouri.

Other molecular modeling techniques can also be employed in  
accordance with this invention. See, e.g., Cohen et al., (1990) *J. Med. Chem.*  
33: 883-894. See also, Navia & Murcko, (1992) *Current Opinions in Structural*

*Biology 2*: 202-210; U.S. Patent No. 6,008,033, herein incorporated by reference.

Once a compound has been designed or selected by the above methods, the efficiency with which that compound can bind to Tie2K can be tested and optimized by computational evaluation. For example, a compound that has been designed or selected to function as a Tie2K modulator should also preferably traverse a volume not overlapping that occupied by the binding site when it is bound to its native ligand. An effective Tie2K modulator should preferably demonstrate a relatively small difference in energy between its bound and free states (i.e., a small deformation energy of binding). Thus, the most efficient Tie2K modulators should preferably be designed with a deformation energy of binding of not greater than about 10 kcal/mole, preferably, not greater than 7 kcal/mole. Tie2K modulators can interact with the enzyme in more than one conformation that is similar in overall binding energy. In those cases, the deformation energy of binding is taken to be the difference between the energy of the free compound and the average energy of the conformations observed when the modulator binds to the enzyme.

A compound designed or selected as binding to Tie2K can be further computationally optimized so that in its bound state it would preferably lack repulsive electrostatic interaction with the target enzyme. Such non-complementary (e.g., electrostatic) interactions include repulsive charge-charge, dipole-dipole and charge-dipole interactions. Specifically, the sum of all electrostatic interactions between the modulator and the enzyme when the

modulator is bound to Tie2K, preferably make a neutral or favorable contribution to the enthalpy of binding.

Specific computer software is available in the art to evaluate compound deformation energy and electrostatic interaction. Examples of programs

5 designed for such uses include:

1. Gaussian 98, which is available from Gaussian, Inc., Pittsburgh, Pennsylvania;

2. AMBER™ program, version 6.0, which is available from the University of California at San Francisco;

10 3. QUANTA™ program, which is available from Molecular Simulations, Inc., San Diego, California;

4. CHARMM® program, which is available from Molecular Simulations, Inc., San Diego, California; and

15 4. Insight II® program, which is available from Molecular Simulations, Inc., San Diego, California.

These programs can be implemented using a suitable computer system, for instance, a Silicon Graphics workstation, IRIS 4D/35 or IBM RISC/6000 workstation model 550. Other hardware systems and software packages will be apparent to those skilled in the art after review of the  
20 disclosure of the present invention presented herein.

Once a Tie2K modulating compound has been optimally selected or designed, as described above, substitutions can then be made in some of its atoms or side groups in order to improve or modify its binding properties. Generally, initial substitutions are conservative, i.e., the replacement group

will have approximately the same size, shape, hydrophobicity and charge as the original group. It should, of course, be understood that components known in the art to alter conformation should be avoided. Such substituted chemical compounds can then be analyzed for efficiency of fit to a Tie2K  
5 binding site using the same computer-based approaches described in detail above.

10 IV.B. Method of Screening for Chemical and Biological Modulators of  
the Biological Activity of Tie2

Once a candidate modulator compound is designed and tested as described above, it can be further tested in a screening assay. A representative method of screening candidate substances for their ability to modulate the biological activity of Tie2K comprises: (a) providing a library of  
15 test samples; (b) contacting a crystalline form of a cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide with each test sample; (c) detecting an interaction between a test sample and the crystalline form of cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide; (d) identifying a test sample that interacts with the cytoplasmic Tie2 receptor tyrosine kinase domain  
20 polypeptide; and (e) isolating a test sample that interacts with the cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide.

A candidate substance identified according to the screening assay described herein has an ability to modulate the biological activity of the Tie2 and Tie2K polypeptides. Such a candidate compound has utility in the

treatment of disorders and conditions associated with the biological activity of the Tie2 and Tie2K polypeptides, including vascular dysmorphogenesis. Candidate compounds can be hydrophilic, hydrophobic, polycyclic molecules, or any combination thereof, and are typically about 500-1,000 daltons in  
5 molecular weight.

In a cell-free system, the method can comprise establishing a control system comprising a Tie2 or Tie2K polypeptide and a ligand which is capable of binding to the polypeptide; establishing a test system comprising a Tie2 or Tie2K polypeptides, the ligand, and a candidate compound; and determining  
10 whether the candidate compound modulates the activity of the polypeptide by comparison of the test and control systems. A representative ligand comprises a small molecule, and in this embodiment, the biological activity or property screened includes binding affinity.

In another embodiment of the invention, the Tie2 or Tie2K polypeptide  
15 or a catalytic or immunogenic fragment or oligopeptide thereof, can be used for screening libraries of compounds in any of a variety of drug screening techniques. The libraries of compounds preferably comprise compounds designed and tested as described in section IV.A. above. The fragment employed in such screening can be free in solution, affixed to a solid support,  
20 borne on a cell surface, or located intracellularly. The formation of binding complexes between the Tie2 or Tie2K polypeptide and the agent being tested can be measured. In a preferred embodiment, the Tie2 polypeptide has an amino acid sequence of SEQ ID NO: 2. When the Tie2K polypeptide is employed, a preferred embodiment comprises a Tie2K polypeptide having the

amino acid sequence of SEQ ID NO: 4. A mutant Tie2K of the present invention, preferably having the amino acid sequence of SEQ ID NO: 6, can also be employed.

Another technique for drug screening which can be used provides for  
5 high throughput screening of compounds having suitable binding affinity to the protein of interest as described in published PCT application WO 84/03564, herein incorporated by reference. In this method, as applied to a polypeptide of the present invention, large numbers of different small test compounds are synthesized on a solid substrate, such as plastic pins or some other surface.  
10 The libraries of compounds preferably comprise compounds designed and tested as described in section IV.A. above. The test compounds are reacted with the polypeptide, or fragments thereof, and washed. Bound polypeptide is then detected by methods well known in the art. The purified polypeptide can also be coated directly onto plates for use in the aforementioned drug  
15 screening techniques. Alternatively, non-neutralizing antibodies can be used to capture the peptide and immobilize it on a solid support.

In each of the foregoing embodiments, an interaction can be detected spectrophotometrically, radiologically or immunologically. An interaction between a Tie2 or Tie2K polypeptide and a test sample can also be  
20 quantified. Such an interaction can be quantified by determining Tie2 or Tie2K activity.

A screening assay of the present invention can also involve determining the ability of a candidate substance to modulate, i.e. inhibit or promote Tie2 or Tie2K biological activity and preferably, to thereby modulate

the biological activity of Tie2 or Tie2K in target cells. Target cells can be either naturally occurring cells known to contain a polypeptide gene product of the present invention or transfected cells. The test samples can further comprise a cell or cell line that expresses the Tie2 or Tie2K polypeptide gene product of the present invention, for example, *Xenopus* oocytes expressing a foreign Tie2 or Tie2K. Such cell lines can be mammalian, or human, or they can from another organism, including but not limited to yeast. Representative assays include genetic screening assays and molecular biology screens such as a yeast two-hybrid screen that will effectively identify genes related to angiogenesis, vasculogenesis or a cellular process related to these biological phenomena. One version of the yeast two-hybrid system has been described (Chien et al., (1991) *Proc. Natl. Acad. Sci. USA*, 88: 9578-82) and is commercially available from Clontech (Palo Alto, California).

As is well known in the art, a screening assay can provide a cell under conditions suitable for testing the modulation of the biological activity of a Tie2 or Tie2K polypeptide. These conditions include but are not limited to pH, temperature, tonicity, the presence of relevant metabolic factors (e.g., metal ions such as for example  $Mg^{++}$ , growth factors, or angiopoietins), and relevant modifications to a Tie2 or Tie2K polypeptide such as phosphorylation. A Tie2 or Tie2K polypeptide of the present invention can be expressed and utilized in a prokaryotic or eukaryotic cell. The host cell can also be fractionated into sub-cellular fractions where a structure of interest can be found. For example, cells expressing the Tie2 or Tie2K polypeptide can be fractionated into the

nuclei, the endoplasmic reticulum, vesicles, or the membrane surfaces of the cell.

In accordance with the present invention there is also provided a rapid and high throughput screening method that relies on the methods described  
5 above. This screening method comprises separately contacting each of a plurality of substantially identical samples. In such a screening method the plurality of samples preferably comprises more than about  $10^4$  samples, or more preferably comprises more than about  $5 \times 10^4$  samples.

10 V. Design, Preparation and Structural Analysis of Additional Tie2 and Tie2K Mutants and Structural Equivalents

The present invention also provides for the generation of Tie2 and Tie2K mutants and the ability to solve the crystal structures of those that crystallize. More particularly, through the provision of the three-dimensional  
15 structure of Tie2K, desirable sites for mutation can be identified.

The structure coordinates of Tie2K mutants provided in accordance with the present invention also facilitate the identification of related proteins or enzymes analogous to Tie2K in function, structure or both, (for example, FGFR), which can lead to novel therapeutic modes for treating or preventing a  
20 range of disease states.

V.A. Sterically Similar Compounds

A further aspect of the present invention is that other sterically similar compounds can be formulated to mimic the key portions of the Tie2K



structure. Such compounds can be used in the same manner as the peptides of the present invention and hence are also functional equivalents. The generation of a structural functional equivalent can be achieved by the techniques of modeling and chemical design known to those of skill in the art and described herein. Modeling and chemical design of Tie2K structural equivalents can be based on the structure coordinates of the present invention. It will be understood that all such sterically similar constructs fall within the scope of the present invention.

#### 10        V.B. Tie2 Polypeptides

The generation of chimeric Tie2 polypeptides is also an aspect of the present invention. Such a chimeric polypeptide can contain the Tie2K polypeptide or a portion of Tie2K, which can be fused to a candidate polypeptide or a suitable region of the candidate polypeptide, for example FGF. Throughout the instant disclosure it is intended that the term "mutant" encompass not only the polypeptide of Tie2K but chimeric proteins generated using Tie2K as well. It is intended that the following discussion of Tie2K mutants applies *mutatis mutandis* to chimeric Tie2 and Tie2K polypeptides and to structural equivalents thereof.

20        In accordance with the present invention, a mutation can be directed to a particular site or combination of sites of wild-type Tie2K, i.e., an accessory binding site, the active site, or an autophosphorylation site can be chosen for mutagenesis. Similarly, a residue having a location on, at or near the surface of the polypeptide can be replaced, resulting in an altered surface charge of

one or more charge units, as compared to the wild-type Tie2 and Tie2K. Alternatively, an amino acid residue in Tie2 or Tie2K can be chosen for replacement based on its hydrophilic or hydrophobic characteristics.

Such mutants can be characterized by any one of several different  
5 properties as compared with wild-type Tie2K. For example, such mutants can have an altered surface charge of one or more charge units, or have an increase in overall stability. Or such mutants can have an altered substrate specificity in comparison with, or a higher specific activity than, wild-type Tie2 and Tie2K.

10 The mutants of Tie2K prepared by this invention can be prepared in a number of ways. For example, the wild-type sequence of Tie2 or Tie2K can be mutated in those sites identified using this invention as desirable for mutation, by means of oligonucleotide-directed mutagenesis or other conventional methods, e.g. deletion. Alternatively, mutants of Tie2 or Tie2K  
15 can be generated by the site-specific replacement of a particular amino acid with an unnaturally occurring amino acid. In addition, Tie2 or Tie2K mutants can be generated through replacement of an amino acid residue, for example, a particular cysteine or methionine residue, with selenocysteine or selenomethionine. This can be achieved by growing a host organism capable  
20 of expressing either the wild-type or mutant polypeptide on a growth medium depleted of either natural cysteine or methionine (or both) but enriched in selenocysteine or selenomethionine (or both).

Mutations can be introduced into a DNA sequence coding for Tie2K using synthetic oligonucleotides. These oligonucleotides contain nucleotide

sequences flanking the desired mutation sites. Mutations can be generated in the full-length DNA sequence of Tie2K or in any sequence coding for polypeptide fragments of Tie2K.

According to the present invention, a mutated Tie2K DNA sequence  
5 produced by the methods described above, or any alternative methods known in the art, can be expressed using an expression vector. An expression vector, as is well known in the art, typically includes elements that permit autonomous replication in a host cell independent of the host genome, and one or more phenotypic markers for selection purposes. Either prior to or  
10 after insertion of the DNA sequences surrounding the desired Tie2K mutant coding sequence, an expression vector also will include control sequences encoding a promoter, operator, ribosome binding site, translation initiation signal, and, optionally, a repressor gene or various activator genes and a signal for termination. In some embodiments, where secretion of the produced  
15 mutant is desired, nucleotides encoding a "signal sequence" can be inserted prior to the Tie2K mutant coding sequence. For expression under the direction of the control sequences, a desired DNA sequence must be operatively linked to the control sequences-- i.e., they must have an appropriate start signal in front of the DNA sequence encoding the Tie2K  
20 mutant and maintaining the correct reading frame to permit expression of that sequence under the control of the control sequences and production of the desired product encoded by that Tie2K sequence.

Any of a wide variety of well-known available expression vectors are useful to express the mutated Tie2K coding sequences of this invention.

These include for example, vectors consisting of segments of chromosomal, non-chromosomal and synthetic DNA sequences, such as various known derivatives of SV40, known bacterial plasmids, e.g., plasmids from *E. coli* including col E1, pCR1, pBR322, pMB9 and their derivatives, wider host  
5 range plasmids, e.g., RP4, phage DNAs, e.g., the numerous derivatives of phage  $\lambda$ , e.g., NM 989, and other DNA phages, e.g., M13 and filamentous single stranded DNA phages, yeast plasmids and vectors derived from combinations of plasmids and phage DNAs, such as plasmids which have been modified to employ phage DNA or other expression control sequences.  
10 In the preferred embodiments of this invention, vectors amenable to expression in a baculovirus expression system are employed.

In addition, any of a wide variety of expression control sequences-- sequences that control the expression of a DNA sequence when operatively linked to it-- can be used in these vectors to express the mutated DNA  
15 sequences according to this invention. Such useful expression control sequences, include, for example, the early and late promoters of SV40 for animal cells, the lac system, the trp system the TAC or TRC system, the major operator and promoter regions of phage  $\lambda$ , the control regions of fd coat protein, all for *E. coli*, the promoter for 3-phosphoglycerate kinase or other  
20 glycolytic enzymes, the promoters of acid phosphatase, e.g., Pho5, the promoters of the yeast  $\alpha$ -mating factors for yeast, and other sequences known to control the expression of genes of prokaryotic or eukaryotic cells or their viruses, and various combinations thereof.

A wide variety of hosts are also useful for producing mutated Tie2K polypeptides according to this invention. These hosts include, for example, bacteria, such as *E. coli*, *Bacillus* and *Streptomyces*, fungi, such as yeasts, and animal cells, such as CHO and COS-1 cells, plant cells, insect cells, such as Sf9 cells, and transgenic host cells.

It should be understood that not all expression vectors and expression systems function in the same way to express mutated DNA sequences of this invention and to produce modified Tie2K or Tie2K mutants. Neither do all hosts function equally well with the same expression system. However, one of skill in the art can make a selection among these vectors, expression control sequences and hosts without undue experimentation and without departing from the scope of this invention. For example, an important consideration in selecting a vector will be the ability of the vector to replicate in a given host. The copy number of the vector, the ability to control that copy number, and the expression of any other proteins encoded by the vector, such as antibiotic markers, should also be considered.

In selecting an expression control sequence, a variety of factors should also be considered. These include, for example, the relative strength of the system, its controllability, its compatibility with the DNA sequence encoding the modified Tie2K polypeptide of this invention, particularly with regard to potential secondary structures.

Hosts should be selected by consideration of their compatibility with the chosen vector, the toxicity of the modified Tie2K to them, their ability to express mature products, their ability to fold proteins correctly, their

fermentation requirements, the ease of the purification of the modified Tie2K from them and safety. Within these parameters, one of skill in the art can select various vector/expression control system/host combinations that will produce useful amounts of a mutant Tie2K. A mutant Tie2K produced in these systems can be purified by a variety of conventional steps and strategies, including those used to purify wild-type Tie2K.

Once a Tie2K mutant(s) has been generated in the desired location, i.e., active site, accessory binding site or phosphorylation site, the mutants can be tested for any one of several properties of interest. For example, mutants can be screened for an altered charge at physiological pH. This is determined by measuring the mutant Tie2K isoelectric point (pI) in comparison with that of the wild-type parent. Isoelectric point can be measured by gel-electrophoresis according to the method of Wellner (Wellner, (1971) *Analyt. Chem.* 43: 597). A mutant with an altered surface charge is a Tie2K polypeptide containing a replacement amino acid located at the surface of the enzyme, as provided by the structural information of this invention, and an altered pI.

#### 20      V.C. Generation of an Engineered Tie2 or Tie2K Mutant

In another aspect of the present invention, a unique Tie2 or Tie2K mutant can be generated. Such a mutant can facilitate purification and the study of Tie2's autophosphorylation abilities. Specifically, by mutating tyrosine 897 to phenylalanine, it is possible to obtain an activated Tie2 or

Tie2K polypeptide. By mutating tyrosine 1048 to phenylalanine, it is possible to generate a mutant Tie2 or Tie2K polypeptide that allows for more homogeneous preparations of the polypeptide. Similarly, by mutating serine 1119 to alanine it is possible to generate a Tie2 or Tie2K mutant that allows  
5 for more homogeneous preparations of the polypeptide. These mutations can be present alone or in combination in a single Tie2 or Tie2K polypeptide, and can provide an activated mutant Tie2 or Tie2K polypeptide with enhanced purification properties.

In a preferred embodiment, a mutant Tie2 or Tie2K of the present  
10 invention comprises the nucleic acid sequence shown in SEQ ID NO: 5. More preferably, a mutant Tie2 or Tie2K of the present invention comprises the amino acid sequence shown in SEQ ID NO: 6. Even more preferably, a mutant Tie2 or Tie2K of the present invention comprises three point mutations: tyrosine 897 is mutated to phenylalanine; tyrosine 1048 is mutated  
15 to phenylalanine and serine 1119 is mutated to alanine.

As used in the following discussion, the term "engineered Tie2 or Tie2K mutant" refers to polypeptides having amino acid sequences which contain at least one of the mutations Y897F, Y1048F, or S1119A. The term also refers to Tie2 and Tie2K polypeptides which are capable of exerting a biological  
20 effect in that they comprise all or a part of the amino acid sequence of an engineered Tie2 or Tie2K mutant polypeptide of the present invention, or cross-react with antibodies raised against an engineered Tie2 or Tie2K mutant polypeptide, or retain all or some or an enhanced degree of the biological activity of the engineered Tie2 or Tie2K mutant amino acid

sequence or protein. Such biological activity can include autophosphorylation or immunogenicity.

The term "engineered Tie2 or Tie2K mutant" also includes analogs of an engineered Tie2 or Tie2K mutant polypeptide. By "analog" is intended that a DNA or polypeptide sequence can contain alterations relative to the sequences disclosed herein, yet retain all or some or an enhanced degree of the biological activity of those sequences. Analogs can be derived from genomic nucleotide sequences as are disclosed herein or from other organisms, or can be created synthetically. Those skilled in the art will appreciate that other analogs, as yet undisclosed or undiscovered, can be used to design and/or construct Tie2 or Tie2K mutant analogs. There is no need for an engineered Tie2 or Tie2K mutant polypeptide to comprise all or substantially all of the amino acid sequence of SEQ ID NO: 6. Shorter or longer sequences are anticipated to be of use in the invention; shorter sequences are herein referred to as "segments". Thus, the term "engineered Tie2 or Tie2K mutant" also includes fusion, chimeric or recombinant engineered Tie2 or Tie2K mutant polypeptides and proteins comprising sequences of the present invention. Methods of preparing such proteins are disclosed herein above and are known in the art.

20

#### V.C.1 Sequence Similarity and Identity

As used herein, the term "substantially similar" means that a particular sequence varies from nucleic acid sequence of SEQ ID NO: 5, or the amino acid sequence of SEQ ID NO: 6 by one or more deletions, substitutions, or



additions, the net effect of which is to retain at least some of biological activity of the natural gene, gene product, or sequence. Such sequences include "mutant" or "polymorphic" sequences, or sequences in which the biological activity and/or the physical properties are altered to some degree but retains  
5 at least some or an enhanced degree of the original biological activity and/or physical properties. In determining nucleic acid sequences, all subject nucleic acid sequences capable of encoding substantially similar amino acid sequences are considered to be substantially similar to a reference nucleic acid sequence, regardless of differences in codon sequences or substitution  
10 of equivalent amino acids to create biologically functional equivalents.

V.D. Sequences That are Substantially Identical to an Engineered  
Mutant Tie2K Sequence of the Present Invention

Additionally, nucleic acids that are substantially identical to a nucleic  
15 acid sequence of an engineered Tie2 or Tie2K mutant of the present invention, e.g. allelic variants, genetically altered versions of the gene, etc., bind to an engineered Tie2 or Tie2K mutant sequence under stringent hybridization conditions. By using probes, particularly labeled probes of DNA sequences, one can isolate homologous or related genes. The source of  
20 homologous genes can be any species, e.g. primate species; rodents, such as rats and mice, canines, felines, bovines, equines, yeast, nematodes, etc.

Between mammalian species, e.g. human and mouse, homologs have substantial sequence similarity, i.e. at least 75% sequence identity between nucleotide sequences. Sequence similarity is calculated based on a reference

sequence, which can be a subset of a larger sequence, such as a conserved motif, coding region, flanking region, etc. A reference sequence will usually be at least about 18 nt long, more usually at least about 30 nt long, and can extend to the complete sequence that is being compared. Algorithms for sequence analysis are known in the art, such as BLAST, described in Altschul et al., (1990) *J. Mol. Biol.* 215: 403-10.

Percent identity or percent similarity of a DNA or peptide sequence can be determined, for example, by comparing sequence information using the GAP computer program, available from the University of Wisconsin Geneticist Computer Group. The GAP program utilizes the alignment method of Needleman et al., (1970) *J. Mol. Biol.* 48: 443, as revised by Smith et al., (1981) *Adv. Appl. Math.* 2:482. Briefly, the GAP program defines similarity as the number of aligned symbols (i.e., nucleotides or amino acids) which are similar, divided by the total number of symbols in the shorter of the two sequences. The preferred parameters for the GAP program are the default parameters, which do not impose a penalty for end gaps. See, e.g., Schwartz et al., eds., (1979), Atlas of Protein Sequence and Structure, National Biomedical Research Foundation, pp. 357-358; Gribskov et al., (1986) *Nucl. Acids. Res.* 14: 6745.

The term "similarity" is contrasted with the term "identity". Similarity is defined as above; "identity", however, means a nucleic acid or amino acid sequence having the same amino acid at the same relative position in a given family member of a gene family. Homology and similarity are generally viewed as broader terms than the term identity. Biochemically similar amino

acids, for example leucine/isoleucine or glutamate/aspartate, can be present at the same position-- these are not identical per se, but are biochemically "similar." As disclosed herein, these are referred to as conservative differences or conservative substitutions. This differs from a conservative mutation at the DNA level, which changes the nucleotide sequence without making a change in the encoded amino acid, e.g. TCC to TCA, both of which encode serine.

As used herein, DNA analog sequences are "substantially identical" to specific DNA sequences disclosed herein if: (a) the DNA analog sequence is derived from coding regions of the nucleic acid sequence shown in SEQ ID NO: 5; or (b) the DNA analog sequence is capable of hybridization of DNA sequences of (a) under stringent conditions and which encode a biologically active Tie2 or Tie2K gene product; or (c) the DNA sequences are degenerate as a result of alternative genetic code to the DNA analog sequences defined in (a) and/or (b). Substantially identical analog proteins and nucleic acids will have between about 70% and 80%, preferably between about 81% to about 90% or even more preferably between about 91% and 99% sequence identity with the corresponding sequence of the native protein or nucleic acid. Sequences having lesser degrees of identity but comparable biological activity are considered to be equivalents.

As used herein, "stringent conditions" means conditions of high stringency, for example 6XSSC, 0.2% polyvinylpyrrolidone, 0.2% Ficoll, 0.2% bovine serum albumin, 0.1% sodium dodecyl sulfate, 100 µg/ml salmon sperm DNA and 15% formamide at 68° C. For the purposes of specifying additional

conditions of high stringency, preferred conditions are salt concentration of about 200 mM and temperature of about 45°C. One example of such stringent conditions is hybridization at 4XSSC, at 65°C, followed by a washing in 0.1XSSC at 65°C for one hour. Another exemplary stringent hybridization  
5 scheme uses 50% formamide, 4XSSC at 42°C.

In contrast, nucleic acids having sequence similarity are detected by hybridization under lower stringency conditions. Thus, sequence identity can be determined by hybridization under lower stringency conditions, for example, at 50°C or higher and 0.1XSSC (9 mM NaCl/0.9 mM sodium citrate)  
10 and the sequences will remain bound when subjected to washing at 55°C in 1XSSC.

V.E. Complementarity and Hybridization to an Engineered Tie2 or Tie2K Mutant Sequence

15 As used herein, the term "complementary sequences" means nucleic acid sequences which are base-paired according to the standard Watson-Crick complementarity rules. The present invention also encompasses the use of nucleotide segments that are complementary to the sequences of the present invention. A particular example of a contemplated complementary  
20 nucleic acid segment is an antisense oligonucleotide.

Hybridization can also be used for assessing complementary sequences and/or isolating complementary nucleotide sequences. As discussed above, nucleic acid hybridization will be affected by such conditions as salt concentration, temperature, or organic solvents, in addition to the base

composition, length of the complementary strands, and the number of nucleotide base mismatches between the hybridizing nucleic acids, as will be readily appreciated by those skilled in the art. Stringent temperature conditions will generally include temperatures in excess of about 30°C, typically in excess of about 37°C, and preferably in excess of about 45°C. Stringent salt conditions will ordinarily be less than about 1,000 mM, typically less than about 500 mM, and preferably less than about 200 mM. However, the combination of parameters is much more important than the measure of any single parameter. See, e.g., Wetmur & Davidson, (1968) *J. Mol. Biol.* 31: 349-70. Determining appropriate hybridization conditions to identify and/or isolate sequences containing high levels of homology is well known in the art. See, e.g., Sambrook et al., (1992) Molecular Cloning: A Laboratory Manual, Cold Spring Harbor, New York.

15        V.F. Functional Equivalents of an Engineered Tie2 or Tie2K Mutant  
              Nucleic Acid Sequence of the Present Invention

As used herein, the term "functionally equivalent codon" is used to refer to codons that encode the same amino acid, such as the ACG and AGU codons for serine. Tie2 or Tie2K-encoding nucleic acid sequences comprising  
20    SEQ ID NO: 5 which have functionally equivalent codons are covered by the invention. Thus, when referring to the sequence example presented in SEQ ID NO: 5, applicants contemplate substitution of functionally equivalent codons into the sequence example of SEQ ID NO: 5. Thus, applicants are in possession of amino acid and nucleic acids sequences which include such

substitutions but which are not set forth herein in their entirety for convenience.

It will also be understood by those of skill in the art that amino acid and nucleic acid sequences can include additional residues, such as additional N-  
5 or C-terminal amino acids or 5' or 3' nucleic acid sequences, and yet still be essentially as set forth in one of the sequences disclosed herein, so long as the sequence retains biological protein activity where polypeptide expression is concerned. The addition of terminal sequences particularly applies to nucleic acid sequences which can, for example, include various non-coding  
10 sequences flanking either of the 5' or 3' portions of the coding region or can include various internal sequences, i.e., introns, which are known to occur within genes.

#### V.G. Biological Equivalents

15 The present invention envisions and includes biological equivalents of an engineered Tie2 or Tie2K mutant polypeptide of the present invention. The term "biological equivalent" refers to proteins having amino acid sequences which are substantially identical to the amino acid sequence of an engineered Tie2K mutant of the present invention and which are capable of exerting a  
20 biological effect in that they are capable of being autophosphorylated at residue tyrosine 992, leading to an activated Tie2 or Tie2K polypeptide, or cross-reacting with anti-Tie2 or Tie2K mutant antibodies raised against an engineered mutant Tie2 or Tie2K polypeptide of the present invention.

For example, certain amino acids can be substituted for other amino acids in a protein structure without appreciable loss of interactive capacity with, for example, structures in the nucleus of a cell. Since it is the interactive capacity and nature of a protein that defines that protein's biological functional activity, certain amino acid sequence substitutions can be made in a protein sequence (or the nucleic acid sequence encoding it) to obtain a protein with the same, enhanced, or antagonistic properties. Such properties can be achieved by interaction with the normal targets of the protein, but this need not be the case, and the biological activity of the invention is not limited to a particular mechanism of action. It is thus in accordance with the present invention that various changes can be made in the amino acid sequence of an engineered Tie2 or Tie2K mutant polypeptide of the present invention or its underlying nucleic acid sequence without appreciable loss of biological utility or activity.

Biologically equivalent polypeptides, as used herein, are polypeptides in which certain, but not most or all, of the amino acids can be substituted. Thus, when referring to the sequence example presented in SEQ ID NO: 5, applicants envision substitution of codons that encode biologically equivalent amino acids as described herein into the sequence example of SEQ ID NO: 6. Thus, applicants are in possession of amino acid and nucleic acids sequences which include such substitutions but which are not set forth herein in their entirety for convenience.

Alternatively, functionally equivalent proteins or peptides can be created via the application of recombinant DNA technology, in which changes

in the protein structure can be engineered, based on considerations of the properties of the amino acids being exchanged, e.g. substitution of Ile for Leu. Changes designed by man can be introduced through the application of site-directed mutagenesis techniques, e.g., to introduce improvements to the antigenicity of the protein or to test an engineered Tie2 or Tie2K mutant polypeptide of the present invention in order to modulate autophosphorylation activity, or other activity at the molecular level.

Amino acid substitutions, such as those which might be employed in modifying an engineered Tie2 or Tie2K mutant polypeptide of the present invention are generally, but not necessarily, based on the relative similarity of the amino acid side-chain substituents, for example, their hydrophobicity, hydrophilicity, charge, size, and the like. An analysis of the size, shape and type of the amino acid side-chain substituents reveals that arginine, lysine and histidine are all positively charged residues; that alanine, glycine and serine are all of similar size; and that phenylalanine, tryptophan and tyrosine all have a generally similar shape. Therefore, based upon these considerations, arginine, lysine and histidine; alanine, glycine and serine; and phenylalanine, tryptophan and tyrosine; are defined herein as biologically functional equivalents. Other biologically functionally equivalent changes will be appreciated by those of skill in the art. It is implicit in the above discussion, however, that one of skill in the art can appreciate that a radical, rather than a conservative substitution is warranted in a given situation. Non-conservative substitutions in engineered mutant Tie2 or Tie2K polypeptides of the present



invention, for example SEQ ID NO: 6, are, therefore, an aspect of the present invention.

In making biologically functional equivalent amino acid substitutions, the hydrophobic index of amino acids can be considered. Each amino acid  
5 has been assigned a hydrophobic index on the basis of their hydrophobicity and charge characteristics, these are: isoleucine (+ 4.5); valine (+ 4.2); leucine (+ 3.8); phenylalanine (+ 2.8); cysteine (+ 2.5); methionine (+ 1.9); alanine (+ 1.8); glycine (-0.4); threonine (-0.7); serine (-0.8); tryptophan (-0.9); tyrosine (-1.3); proline (-1.6); histidine (-3.2); glutamate (-3.5); glutamine (-  
10 3.5); aspartate (-3.5); asparagine (-3.5); lysine (-3.9); and arginine (-4.5).

The importance of the hydrophobic amino acid index in conferring interactive biological function on a protein is generally understood in the art (Kyte & Doolittle, (1982), J. Mol. Biol. 157: 105-132) incorporated herein by reference). It is known that certain amino acids can be substituted for other  
15 amino acids having a similar hydrophobic index or score and still retain a similar biological activity. In making changes based upon the hydrophobic index, the substitution of amino acids whose hydrophobic indices are within  $\pm 2$  of the original value is preferred, those which are within  $\pm 1$  of the original value are particularly preferred, and those within  $\pm 0.5$  of the original value are  
20 even more particularly preferred.

It is also understood in the art that the substitution of like amino acids can be made effectively on the basis of hydrophilicity. U.S. Patent No. 4,554,101, incorporated herein by reference, states that the greatest local average hydrophilicity of a protein, as governed by the hydrophilicity of its

adjacent amino acids, correlates with its immunogenicity and antigenicity, i.e. with a biological property of the protein. It is understood that an amino acid can be substituted for another having a similar hydrophilicity value and still obtain a biologically equivalent protein.

5       As detailed in U.S. Pat. No. 4,554,101, the following hydrophilicity values have been assigned to amino acid residues: arginine (+ 3.0); lysine (+ 3.0); aspartate (+ 3.0 $\pm$ 1); glutamate (+ 3.0 $\pm$ 1); serine (+ 0.3); asparagine (+ 0.2); glutamine (+ 0.2); glycine (0); threonine (-0.4); proline (-0.5 $\pm$ 1); alanine (-0.5); histidine (-0.5); cysteine (-1.0); methionine (-1.3); valine (-1.5); leucine (-10 1.8); isoleucine (-1.8); tyrosine (-2.3); phenylalanine (-2.5); tryptophan (-3.4).

In making changes based upon similar hydrophilicity values, the substitution of amino acids whose hydrophilicity values are within  $\pm 2$  of the original value is preferred, those which are within  $\pm 1$  of the original value are particularly preferred, and those within  $\pm 0.5$  of the original value are even 15 more particularly preferred.

While discussion has focused on functionally equivalent polypeptides arising from amino acid changes, it will be appreciated that these changes can be effected by alteration of the encoding DNA, taking into consideration also that the genetic code is degenerate and that two or more codons can 20 code for the same amino acid.

Thus, it will also be understood that this invention is not limited to the particular amino acid and nucleic acid sequences of SEQ ID NOs: 5 and 6. Recombinant vectors and isolated DNA segments can therefore variously include an engineered Tie2 or Tie2K mutant polypeptide-encoding region

itself, include coding regions bearing selected alterations or modifications in the basic coding region, or include larger polypeptides which nevertheless comprise Tie2 or Tie2K mutant polypeptide-encoding regions or can encode biologically functional equivalent proteins or polypeptides which have variant amino acid sequences. Biological activity of an engineered Tie2 or Tie2K mutant polypeptide can be determined, for example, by phosphorylation assays known to those of skill in the art.

The nucleic acid segments of the present invention, regardless of the length of the coding sequence itself, can be combined with other DNA sequences, such as promoters, enhancers, polyadenylation signals, additional restriction enzyme sites, multiple cloning sites, other coding segments, and the like, such that their overall length can vary considerably. It is therefore contemplated that a nucleic acid fragment of almost any length can be employed, with the total length preferably being limited by the ease of preparation and use in the intended recombinant DNA protocol. For example, nucleic acid fragments can be prepared which include a short stretch complementary to a nucleic acid sequence set forth in SEQ ID NO: 5, such as about 10 nucleotides, and which are up to 10,000 or 5,000 base pairs in length, with segments of 3,000 being preferred in certain cases. DNA segments with total lengths of about 4,000, 3,000, 2,000, 1,000, 500, 200, 100, and about 50 base pairs in length are also useful.

The DNA segments of the present invention encompass biologically functional equivalents of engineered Tie2 or Tie2K mutant polypeptides. Such sequences can arise as a consequence of codon redundancy and functional

equivalency that are known to occur naturally within nucleic acid sequences and the proteins thus encoded. Alternatively, functionally equivalent proteins or polypeptides can be created via the application of recombinant DNA technology, in which changes in the protein structure can be engineered, 5 based on considerations of the properties of the amino acids being exchanged. Changes can be introduced through the application of site-directed mutagenesis techniques, e.g., to introduce improvements to the antigenicity of the protein or to test variants of an engineered Tie2 or Tie2K mutant of the present invention in order to examine the degree of 10 autophosphorylation, or other activity at the molecular level. Various site-directed mutagenesis techniques are known to those of skill in the art.

The invention further encompasses fusion proteins and peptides wherein an engineered Tie2 or Tie2K mutant coding region of the present invention is aligned within the same expression unit with other proteins or 15 peptides having desired functions, such as for purification or immunodetection purposes.

Recombinant vectors form important further aspects of the present invention. Particularly useful vectors are those in which the coding portion of the DNA segment is positioned under the control of a promoter. The promoter 20 can be that naturally associated with a Tie2 gene, as can be obtained by isolating the 5' non-coding sequences located upstream of the coding segment or exon, for example, using recombinant cloning and/or PCR technology and/or other methods known in the art, in conjunction with the compositions disclosed herein.

in other embodiments, certain advantages will be gained by positioning the coding DNA segment under the control of a recombinant, or heterologous, promoter. As used herein, a recombinant or heterologous promoter is a promoter that is not normally associated with a Tie2 gene in its natural environment. Such promoters can include promoters isolated from bacterial, viral, eukaryotic, or mammalian cells. Naturally, it will be important to employ a promoter that effectively directs the expression of the DNA segment in the cell type chosen for expression. The use of promoter and cell type combinations for protein expression is generally known to those of skill in the art of molecular biology (See, e.g., Sambrook et al., 1992, specifically incorporated herein by reference). The promoters employed can be constitutive or inducible and can be used under the appropriate conditions to direct high level expression of the introduced DNA segment, such as is advantageous in the large-scale production of recombinant proteins or peptides. Appropriate promoter systems contemplated for use in high-level expression include, but are not limited to, the vaccinia virus promoter and, more preferably, a baculovirus promoter.

#### VI. Identification of Reaction Intermediates

The present invention also provides for the development of compounds that can isomerize to short-lived reaction intermediates in the chemical reaction of a substrate, or other compound that binds to Tie2 or Tie2K, or with Tie2 or Tie2K. Thus, the time-dependent analysis of structural changes in Tie2 or Tie2K during its interaction with other molecules is provided. The

reaction intermediates of Tie2 or Tie2K-mediated chemical processes can also be deduced from the reaction product in co-complex with Tie2 or Tie2K. Such information is useful to design improved analogues of any known Tie2 or Tie2K modulators, or to design novel classes of modulators based on the  
5 reaction intermediates of the Tie2 or Tie2K polypeptide and the polypeptide-modulator co-complex. This provides a novel route for designing Tie2 or Tie2K modulators with both high specificity and stability.

Another approach provided by the present invention, is to screen computationally small molecule databases for chemical entities or compounds  
10 that can bind in whole, or in part, to the Tie2 or Tie2K polypeptide. In this screening, the quality of fit of such entities or compounds to the binding site can be judged either by shape complementarity or by estimated interaction energy (Meng et al., (1992) *J. Comb. Chem.* 13: 505-524).

15 VII. The Role of the Three-Dimensional Structure of Tie2K in Solving Additional Tie2K Crystals

Because Tie2K can crystallize in more than one crystal form (four representative forms were generated in the present invention), the structure coordinates of Tie2K, or portions thereof, as provided by the present invention  
20 are particularly useful to solve the structure of other crystal forms of Tie2K. They can also be used to solve the structure of Tie2K mutants (such as those prepared as disclosed in Section V above), Tie2K co-complexes, or of the crystalline form of any other protein with significant amino acid sequence homology to any functional domain of Tie2K.

VII.A. Determining the Three-Dimensional Structure of a Polypeptide  
Using the Three-Dimensional Structure of Tie2K as a Template  
in Molecular Replacement

5           One method that can be employed for the purpose of solving additional Tie2K crystal structures, which was used to solve the three-dimensional structure of Tie2K in the present invention, is molecular replacement. In the molecular replacement method, the unknown crystal structure, whether it is another crystal form of Tie2K, i.e. a Tie2K mutant or a Tie2K polypeptide  
10   complexed with another compound (a "co-complex"), or the crystal of some other protein with significant amino acid sequence homology to any functional region of Tie2K, can be determined using the Tie2K structure coordinates provided in Tables 2-5. This method provides an accurate structural form for the unknown crystal more quickly and efficiently than attempting to determine  
15   such information *ab initio*.

          In addition, in accordance with this invention, Tie2K mutants can be crystallized in complex with known Tie2K modulators. The crystal structures of a series of such complexes can then be solved by molecular replacement and compared with that of wild-type Tie2K. Potential sites for modification  
20   within the various binding sites of the enzyme can thus be identified. This information provides an additional tool for determining the most efficient binding interactions, for example, increased hydrophobic interactions, between Tie2K and a chemical entity or compound.

All of the complexes referred to in the instant disclosure can be studied using well-known X-ray diffraction techniques (See, e.g., Blundell & Johnson (1985) *Methods in Enzymology*, 114A & 115B, Wyckoff et al., eds., Academic Press) and can be refined using computer software, such as the X-PLOR™ program (Yale University, © 1992, available from Molecular Simulations, Inc., San Diego, California). This information can thus be used to optimize known classes of Tie2K modulators, and more importantly, to design and synthesize novel classes of Tie2K modulators.

10

#### Laboratory Examples

The following Laboratory Examples have been included to illustrate preferred modes of the invention. Certain aspects of the following Laboratory Examples are described in terms of techniques and procedures found or contemplated by the present inventors to work well in the practice of the invention. These Laboratory Examples are exemplified through the use of standard laboratory practices of the inventors. In light of the present disclosure and the general level of skill in the art, those of skill will appreciate that the following Laboratory Examples are intended to be exemplary only and that numerous changes, modifications and alterations can be employed without departing from the spirit and scope of the invention.

20

#### Laboratory Example 1

##### Protein Expression

The cytoplasmic domain of Tie2 was cloned from a human kidney



cDNA library (Clontech, Palo Alto, California) by PCR. The sequence was identical to that reported in GENBANK (L06139). The coding region corresponding to residues 808-1124 was subcloned into a pFASTBAC1™ (Gibco BRL, Rockville, Maryland) expression vector by PCR. The N-terminal primer included an Sst1 restriction site and a methionine start codon followed by six histidine codons. The C-terminal primer included a stop codon and an Xho1 restriction site. The PCR product was cloned into the Sst1/Xho1 site of pFASTBAC1™. All restriction enzymes were from either New England Biolabs (Beverly, Massachusetts) or GibcoBRL (Rockville, Maryland) and used as suggested by the supplier. The Tie2K construct was transfected into *Spodoptera frugiperda* (Sf9) cells, single plaques were isolated, and high titer stocks were generated. Sf9 cells, in a 36L fermentor, were infected at a multiplicity of infection of 5 for 72 hours and harvested by centrifugation at 3000rpm for 20 minutes.

## Laboratory Example 2

### Protein Purification

Cells from 12L of culture (~200g of wet cell paste) were resuspended in 1200mL of 50 mM HEPES (pH 8), 200 mM NaCl, and 20 mM imidazole and were disrupted using a Polytron® homogenizer (Brinkmann Instruments, Westbury, New York) and by sonication. The homogenate was centrifuged for 40 minutes at 12,500 rpm (Sorvall GSA rotor, available from Kendro Laboratory Products, Newtown, Connecticut). The supernatant was filtered (1.2 micron cartridge filter) and was loaded onto a nickel-chelating column (70mL bed volume, Chelating SEPHAROSE™ FF, Pharmacia, Peapack, New

Jersey) at 20mL/min. Protein was eluted with a 10 column volume linear gradient between 20 and 300 mM imidazole in 50 mM HEPES (pH 8), 200 mM NaCl. 25mL column fractions were collected and analyzed by SDS PAGE. Tie2K protein was pooled and loaded directly onto a hydroxylapatite column having 40mL bed volume (Type I ceramic hydroxylapatite available from BioRad, Inc., of Hercules, California) at 20mL/min. A linear gradient was run from 0 to 100 mM potassium phosphate in 20 mM Tris-HCl (pH 8), 50 mM NaCl, 5 mM DTT, and 5% glycerol. 10mL column fractions were collected and analyzed by SDS PAGE. The Tie2K containing fractions were diluted 1:1 with 20 mM Tris-HCl (pH 8), 5 mM DTT, and 5% glycerol, loaded onto an anion exchange column (35mL bed volume, Q-SEPHAROSE™ HP, Pharmacia, Peapack, New Jersey) at 10mL/min and eluted with a 0-600 mM NaCl gradient. 5mL fractions were collected and analyzed by SDS PAGE and mass spectrometry. Tie2K was pooled based upon SDS PAGE and mass spectrometry analysis (>95% purity) and stored at -80°C. Typically Tie2 eluted in 2 to 3 discrete peaks, reflecting different mixes of phosphorylation states.

### Laboratory Example 3

#### *In vitro* Autophosphorylation for Mass Spectrometry

Wild-type and mutant Tie2K were incubated with 2 mM ATP and 10 mM MgCl<sub>2</sub> for 30 minutes at room temperature in 25 mM HEPES pH 7.5, 150 mM NaCl and 10 mM DTT. Samples were flash frozen in a dry ice/ethanol bath and stored at -180° C until they could be analyzed by mass spectrometry.

#### Laboratory Example 4

##### *In vitro* Kinase Assay

10 nM non-activated or pre-activated Tie2K was used to phosphorylate  
5 1  $\mu$ M of a peptide substrate (Biotin-Ahx-LEARLVAYEGWVAGKKK-NH<sub>2</sub>,  
synthesized by SynPep Corp., Dublin, California) (SEQ ID NO: 13) in the  
presence of 80  $\mu$ M ATP, 10 mM MgCl<sub>2</sub>, 1 mM DTT, 0.1 mg/ml BSA, and 0.1  
M pH 7.5. The reaction was carried out at room temperature for 30 minutes,  
and stopped by the addition of 50 mM EDTA. 1.2  $\mu$ g/ml Streptavidin-APC  
10 (Molecular Probes, Eugene, Oregon) and 0.15  $\mu$ g/ml Eu- $\alpha$ -pY (EG&G Wallac,  
Gaithersburg, Maryland) in the presence of 0.1 mg/ml BSA, 0.1 M HEPES  
pH7.5 were added and the reactions incubated for 10 min at room  
temperature. Streptavidin-APC and Eu- $\alpha$ -pY bind to the phosphorylated  
peptides to form a complex, allowing fluorescent energy transfer from Eu to  
15 APC. The plate was read on a VICTOR™ plate reader (EG&G Wallac,  
Gaithersburg, Maryland) in time resolved fluorescence mode by exciting at  
340 nm and reading the emission at 665 nm.

#### Laboratory Example 5

##### Protein Digestion for Mass Spectrometry

20 Trypsin digestions of 200-1000 picomoles of Tie2K were carried out in  
50 mM Tris pH 8.5, 1 mM CaCl<sub>2</sub>, and 10 % acetonitrile. In some instances,  
Tie2K was reduced and alkylated with DTT and 4-vinylpyridine prior to  
digestion. Digestion proceeded at 37° C for 12-18 hours.

Laboratory Example 6Mass Spectrometry: LCMS

Mass measurements of intact protein were determined using liquid chromatography mass spectrometry (LCMS). Protein samples were initially  
5 desalted on a Poros R2/H column (PerSeptive Biosystems; Framingham, Massachusetts). Effluent from the desalting column was directed to a SCIEX API III™ mass spectrometer (PE Sciex, Concord, Ontario, Canada) and spectra were acquired in positive ion mode with electrospray ionization. Intact  
10 protein mass values were obtained from the reconstructed mass spectra that were generated from the processed data. Assignment of phosphorylation states were made by identifying masses that were multiples of 80 Da higher than the expected mass of Tie2K.

15

Laboratory Example 7Mass Spectrometry: nanoES MS

Nanoelectrospray ionization (nanoES) MS on a Q-TOF instrument from Micromass (Manchester, United Kingdom) was used to map phosphorylation sites after trypsin digestion. Sample was introduced to the MS with either  
20 static nanoES using a pulled capillary tip (Mann) or capillary LCMS/MS. The LC system was from LC Packings of San Francisco, California, and comprised the FAMOS™ autosampler and the ULTIMATE™ solvent delivery pump. Separation was carried out on a 75µm I.D. C<sub>18</sub> PepMap column, also from LC Packings (San Francisco, California). The Q-TOF is capable of data  
25 dependent ion selection for collision-induced fragmentation.

Two sample preparation approaches were used to map the phosphorylation sites. In the first approach, phosphorylated peptides were isolated from nonphosphorylated peptides using Ga(III) immobilized metal affinity chromatography (IMAC). Briefly, an aliquot of the trypsin digest was  
5 acidified and loaded onto an IMAC microcolumn charged with Ga(III). The column was then washed with 0.1% acetic acid/ 30% acetonitrile to remove non-phosphorylated peptides. Retained peptides were then eluted with 0.2 M sodium phosphate, pH 8.2 and directly applied to a microcolumn packed with POROS™ R2/H reverse phase media, available from PerSeptive Biosystems,  
10 of Framingham, Massachusetts. Bound peptides were washed with 0.1 % formic acid and then eluted directly into a nanoelectrospray capillary tip. Static nanoESI was used to acquire MS and MS/MS spectra of the purified peptides. Phosphorylated residues were identified from MS/MS data.

In a second approach, the Tie2K trypsin digest was analyzed by  
15 capillary LCMS/MS with data dependent scanning. This data file was then used to conduct a MASCOT™ protein database search (Matrix Science Ltd., London, United Kingdom) that compares uninterpreted MS/MS data to theoretical MS/MS spectra of user specified proteolytic peptides. The spectra were interpreted manually to confirm the assignment.

20

### Laboratory Example 8

#### Crystallization and Data Collection

All four crystal forms of Tie2K were grown by the hanging drop vapor diffusion method in Linbro plates on siliconized cover slips (Hampton

Research, Laguna Niguel, California). The protein (6mg/ml in 20 mM HEPES pH 7.5, 300 mM NaCl, 5 mM DTT) was mixed with an equal volume of reservoir (typically 2 $\mu$ L + 2 $\mu$ L drops) and incubated at 22°C. The reservoir (500 $\mu$ L) for crystal forms I and II was 2.5% PEG12000 (Fluka Chemie AG, 5 Buchs, Switzerland), 2.5% glycerol (Gibco BRL, Rockville, Maryland), 100 mM HEPES pH 7.5 (Sigma, St. Louis, Missouri), and 10 mM spermidine (Sigma, St. Louis, Missouri). The reservoir (500 $\mu$ L) for crystal form III was 100 mM HEPES pH 7.5 (Sigma, St. Louis, Missouri), 100 mM KCl (Sigma, St. Louis, Missouri), and 10% isopropanol (EM Science) while the reservoir (500 $\mu$ L) for 10 crystal form IV was 100 mM HEPES pH 7.5 (Sigma, St. Louis, Missouri) and 1.5 M NaCl (Sigma, St. Louis, Missouri). Crystals belonging to the four different space groups appeared within several days to several weeks and typically grew to ~100x100x10 $\mu$ m in 1-2 months. All 4 crystal forms had similar chunky plate morphologies. Glycerol was added as a cryoprotectant to 15 a final concentration of 25%, over a period of 1 hour at 22°C, and the crystals, suspended in nylon loops on copper pins (Hampton Research, Laguna Niguel, California), were flash frozen in liquid N<sub>2</sub>.

Data for crystal forms I, II and IV were collected at -180°C at beamline 17-ID on a MAR-CCD in the facilities of the Industrial Macromolecular 20 Crystallography Association Collaborative Access Team (IMCA-CAT) at the Advanced Photon Source (Argonne National Laboratory, Argonne, Illinois) using X-rays with a wavelength of 1.0 Å. These facilities are supported by the companies of the Industrial Macromolecular Crystallography Association through a contract with Illinois Institute of Technology (IIT), executed through

the iIT's Center for Synchrotron Radiation Research and Instrumentation. In all three cases 180° of data was collected using 1° oscillations every 10 seconds. The detector was set to 150 mm. The space group was determined for each crystal form by merging the data from the first 5 oscillations using the HKL2000 software package (Otwinowski, (1993) in *Proceedings of the CCP4 Study Weekend: Data Collection and Processing*. (Sawyer et al., eds.), pp.56-62, SERC Daresbury Laboratory, England.), available from Nonius B.V, Delft, The Netherlands. Entire data sets were processed using the HKL2000 software package (Nonius B.V., Delft, The Netherlands) (Otwinowski, (1993) in *Proceedings of the CCP4 Study Weekend: Data Collection and Processing*. (Sawyer et al., eds.), pp.56-62, SERC Daresbury Laboratory, England). Data for crystal form III was collected at -180°C on an RAXIS IV image plate (Rigaku, Tokyo, Japan). The CuK $\alpha$  X-rays, having a wavelength of 1.54 Å, were generated on a rotating anode, also available from Rigaku, (Tokyo, Japan) operating at 50 KVx100 mA. The space group was determined from a single oscillation using DENZO (HKL Research, Charlottesville, Virginia). 180° of data was collected using 1.5° oscillations every 50 min. The detector was set to 150 mm. The data were processed with DENZO™ (HKL Research, Charlottesville, Virginia) and scaled with SCALEPACK™, (Otwinowski, (1993) in *Proceedings of the CCP4 Study Weekend: Data Collection and Processing*. (Sawyer et al., eds.), pp.56-62, SERC Daresbury Laboratory, England.) also available from HKL Research, Charlottesville, Virginia.

Laboratory Experiment 9Structure Determination and Refinement

The structure of crystal form I was solved first and subsequently used to solve the other three crystal forms. The structure was solved by molecular replacement using CNS (Brunger et al., (1998) *Acta. Crystallogr.* D54: 905-921.) and FGFR1 as a search model (molecule 1 of PDB entry 1FGK) (Mohammadi et al., (1996) *Cell* 86: 577-87.). The search model contained FGFR1 residues 464-485, 491-500, 506-578, 592-647 and 651-761. Residues not conserved between FGFR1 and Tie2 were truncated to alanine in the model. Rotation and translation searches were carried out using data between 10.0-4.0 Å. For the rotation function, the real space method was used with a minimum Patterson vector length of 5 Å. For the translation search, a general translation function with fastf2f2 target was used. The correct solutions were the top two peaks in both the rotation and translation functions and had correlation coefficients of 0.38 and 0.36. Rigidbody refinement of the two molecules in the asymmetric unit gave an R-factor of 49% using data from 10-4.0 Å. Additional rigid body refinement, using data between 10-3.0 Å, and allowing the 2 domains of the protein to refine independently, dropped the R-factor to 45%. Multiple rounds of model building and refinement were carried out using the AUTOBUILD mode of QUANTA™ (Release 4.0) and CNS, both available from Molecular Simulations, Inc., San Diego, California, using maximum likelihood targets based on the amplitudes. The electron density, generated from the rigidbody solution, allowed placement of most of the side chains from the original



model. When the electron density resolution was extended to the limit of the diffraction, density for portions of the protein not included in the original model could be seen. Additional residues and water molecules were positioned manually in the electron density. Starting with these atomic coordinates, a  
5 diffraction pattern was calculated and compared to the experimental data. The difference between the calculated and experimentally determined diffraction patterns was monitored by the value of the R-factor. The refinement of the structural model necessitates adjustments of atomic positions to minimize the R-factor, where a value of about 20% is typical for a  
10 good quality protein structure. The overall structure was confirmed by a composite simulated-annealing omit map calculated with CNS. The map was generated by sequentially omitting 8% of the protein atoms, carrying out simulated annealing refinement at 1000°C and calculating a  $2F_o - F_c$  electron density map. In the final model residues 813, 858, 860, 867, 997, 1099 and  
15 1119 were modeled as alanine in all four crystal forms due to a lack of side chain density. Analysis of the structure with PROCHECK (Laskowski et al., (1993) *J. Appl. Crystallogr.* 26: 283-291) indicated that all main chain torsions fall within the allowed regions of the Ramachandran plot.

For crystal forms II, III and IV, the final refined model for crystal form I  
20 was used as a search model. Molecular replacement was carried out using CNS using data between 10-4.0 Å. The correlation coefficients were 0.45/0.49, 0.69, and 0.72 for crystal forms II, III and IV, respectively. The R-factor, following rigid body refinement (10-3.0 Å), for the 3 molecular replacement solutions was 38%, 32% and 31%, respectively. Small

differences in the positions of loops and surface exposed side chains were observed and manually rebuilt with the QUANTA™ software program. Waters were added manually.

5

### References

The references listed below as well as all references cited in the specification are incorporated herein by reference to the extent that they supplement, explain, provide a background for or teach methodology,  
10 techniques and/or compositions employed herein.

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U.S. Patent No. 5,872,011

U.S. Patent No. 6,008,033

5 WO 84/03564

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TABLE 1

## CRYSTAL AND DATA STATISTICS

Crystal Form	I	II	III	IV
Space Group	P2 <sub>1</sub>	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	C222 <sub>1</sub>
Unit cell a (Å)	66	79	52	95
Unit cell b (Å)	92	92	77	114
Unit cell c (Å)	70	109	79	78
Unit cell β (°)	108	90	90	90
Mol/asu	2	2	1	1
Resolution (Å)	2.2	2.5	2.2	2.1
R <sub>sym</sub> <sup>a</sup> (%)	7.5	11	7.9	7.8
Completeness (%)	96	98	99	98
R <sub>cryst</sub> <sup>b</sup> (%)	19	21	20	21
R <sub>free</sub> <sup>c</sup> (%)	23	26	23	24
Number of non-hydrogen protein atoms	4766	4766	2368	2375
Number of solvent molecules	361	188	170	200
RMS deviations from ideal				
Bond lengths (Å)	0.0058	0.0063	0.0064	0.0060
Bond angles (°)	1.15	1.16	1.19	1.15

<sup>a</sup>R<sub>sym</sub> =  $\sum_{hkl} |I - \langle I \rangle| / \sum_{hkl} I$ , where I is the observed intensity and  $\langle I \rangle$  is the average intensity from observations of symmetry-related reflections.

<sup>b</sup>R<sub>cryst</sub> =  $\sum_{hkl} ||F_{obs}| - |F_{calc}|| / \sum_{hkl} |F_{obs}|$ , where F<sub>obs</sub> and F<sub>calc</sub> are the observed and calculated structure factor amplitudes, respectively, for the hkl reflections.

<sup>c</sup>R<sub>free</sub> is calculated for a set of reflections that were not included in atomic refinement.

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TABLE 2

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

ATOM	ATOM TYPE	RESIDUE	PROTEIN #	#	X	Y	Z	OCC	B
1	N	ALA	A	813	-13.576	-9.268	4.635	1.00	65.55
2	CA	ALA	A	813	-12.61	-9.129	5.767	1.00	65.19
3	C	ALA	A	813	-13.338	-8.775	7.064	1.00	64.73
4	O	ALA	A	813	-13.069	-7.74	7.673	1.00	64.66
5	CB	ALA	A	813	-11.573	-8.058	5.44	1.00	65.12
6	N	THR	A	814	-14.254	-9.644	7.486	1.00	64.03
7	CA	THR	A	814	-15.019	-9.409	8.709	1.00	62.98
8	C	THR	A	814	-14.925	-10.58	9.68	1.00	62.48
9	O	THR	A	814	-15.033	-11.743	9.288	1.00	62.26
10	CB	THR	A	814	-16.508	-9.167	8.403	1.00	62.61
11	OG1	THR	A	814	-16.633	-8.114	7.442	1.00	61.68
12	CG2	THR	A	814	-17.252	-8.773	9.668	1.00	62.28
13	N	ILE	A	815	-14.721	-10.262	10.953	1.00	61.64
14	CA	ILE	A	815	-14.626	-11.284	11.985	1.00	60.62
15	C	ILE	A	815	-15.838	-11.189	12.906	1.00	59.63
16	O	ILE	A	815	-16.081	-10.16	13.538	1.00	59.84
17	CB	ILE	A	815	-13.329	-11.128	12.806	1.00	60.93
18	CG1	ILE	A	815	-12.118	-11.269	11.878	1.00	61.04
19	CG2	ILE	A	815	-13.279	-12.179	13.918	1.00	60.94
20	CD1	ILE	A	815	-10.781	-11.169	12.573	1.00	61.76
21	N	TYR	A	816	-16.6	-12.273	12.975	1.00	58.21
22	CA	TYR	A	816	-17.792	-12.3	13.808	1.00	56.64
23	C	TYR	A	816	-17.527	-13.091	15.075	1.00	53.88
24	O	TYR	A	816	-16.572	-13.863	15.144	1.00	53.78
25	CB	TYR	A	816	-18.959	-12.924	13.036	1.00	59.01
26	CG	TYR	A	816	-19.08	-12.42	11.618	1.00	60.82
27	CD1	TYR	A	816	-18.2	-12.858	10.629	1.00	61.99
28	CD2	TYR	A	816	-20.051	-11.478	11.27	1.00	61.64
29	CE1	TYR	A	816	-18.279	-12.37	9.326	1.00	62.96
30	CE2	TYR	A	816	-20.139	-10.981	9.968	1.00	62.65
31	CZ	TYR	A	816	-19.249	-11.434	9.004	1.00	63.3
32	OH	TYR	A	816	-19.326	-10.95	7.72	1.00	64.32
33	N	PRO	A	817	-18.367	-12.899	16.098	1.00	51.64
34	CA	PRO	A	817	-19.502	-11.972	16.051	1.00	50.2
35	C	PRO	A	817	-19.073	-10.51	16.135	1.00	49.16
36	O	PRO	A	817	-17.97	-10.197	16.591	1.00	48.82
37	CB	PRO	A	817	-20.334	-12.397	17.257	1.00	50.26
38	CG	PRO	A	817	-19.277	-12.814	18.238	1.00	50.15



TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

39	CD	PRO	A	817	-18.346	-13.635	17.374	1.00	50.65
40	N	VAL	A	818	-19.944	-9.619	15.679	1.00	48.08
41	CA	VAL	A	818	-19.676	-8.193	15.74	1.00	46.39
42	C	VAL	A	818	-19.935	-7.799	17.185	1.00	45.69
43	O	VAL	A	818	-21.007	-8.076	17.724	1.00	45.5
44	CB	VAL	A	818	-20.629	-7.391	14.82	1.00	46.96
45	CG1	VAL	A	818	-20.517	-5.904	15.122	1.00	47.14
46	CG2	VAL	A	818	-20.287	-7.658	13.364	1.00	46.49
47	N	LEU	A	819	-18.954	-7.173	17.819	1.00	44.53
48	CA	LEU	A	819	-19.113	-6.768	19.202	1.00	44.46
49	C	LEU	A	819	-19.436	-5.284	19.286	1.00	44.76
50	O	LEU	A	819	-18.961	-4.49	18.472	1.00	45.45
51	CB	LEU	A	819	-17.835	-7.064	19.987	1.00	43.91
52	CG	LEU	A	819	-17.35	-8.517	19.993	1.00	43.97
53	CD1	LEU	A	819	-16.027	-8.592	20.741	1.00	42.77
54	CD2	LEU	A	819	-18.398	-9.418	20.646	1.00	42.51
55	N	ASP	A	820	-20.25	-4.914	20.267	1.00	44.6
56	CA	ASP	A	820	-20.616	-3.518	20.455	1.00	44.65
57	C	ASP	A	820	-19.658	-2.862	21.441	1.00	43.61
58	O	ASP	A	820	-19.435	-3.367	22.543	1.00	43.24
59	CB	ASP	A	820	-22.049	-3.401	20.975	1.00	46.93
60	CG	ASP	A	820	-22.445	-1.965	21.248	1.00	49.02
61	OD1	ASP	A	820	-22.429	-1.148	20.299	1.00	51.52
62	OD2	ASP	A	820	-22.761	-1.648	22.414	1.00	50.76
63	N	TRP	A	821	-19.105	-1.726	21.036	1.00	42.2
64	CA	TRP	A	821	-18.151	-0.989	21.851	1.00	40.59
65	C	TRP	A	821	-18.578	-0.798	23.303	1.00	40.32
66	O	TRP	A	821	-17.761	-0.919	24.212	1.00	39.65
67	CB	TRP	A	821	-17.864	0.369	21.197	1.00	39.62
68	CG	TRP	A	821	-16.905	1.226	21.957	1.00	38.51
69	CD1	TRP	A	821	-17.212	2.275	22.777	1.00	38.31
70	CD2	TRP	A	821	-15.48	1.095	21.989	1.00	37.17
71	NE1	TRP	A	821	-16.064	2.807	23.319	1.00	38.5
72	CE2	TRP	A	821	-14.986	2.102	22.851	1.00	37.86
73	CE3	TRP	A	821	-14.572	0.226	21.371	1.00	36.2
74	CZ2	TRP	A	821	-13.62	2.263	23.114	1.00	36.99
75	CZ3	TRP	A	821	-13.212	0.384	21.631	1.00	36.89
76	CH2	TRP	A	821	-12.75	1.399	22.497	1.00	36.88
77	N	ASN	A	822	-19.853	-0.514	23.534	1.00	40.74

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

78	CA	ASN	A	822	-20.315	-0.298	24.902	1.00	41.28
79	C	ASN	A	822	-20.392	-1.548	25.766	1.00	40.22
80	O	ASN	A	822	-20.631	-1.459	26.968	1.00	39.55
81	CB	ASN	A	822	-21.663	0.421	24.899	1.00	43.58
82	CG	ASN	A	822	-21.533	1.882	24.517	1.00	46.24
83	OD1	ASN	A	822	-20.827	2.649	25.18	1.00	48.06
84	ND2	ASN	A	822	-22.208	2.275	23.443	1.00	46.98
85	N	ASP	A	823	-20.193	-2.712	25.164	1.00	39.59
86	CA	ASP	A	823	-20.222	-3.951	25.924	1.00	39.46
87	C	ASP	A	823	-18.799	-4.334	26.326	1.00	38.92
88	O	ASP	A	823	-18.587	-5.318	27.024	1.00	38.89
89	CB	ASP	A	823	-20.841	-5.085	25.102	1.00	40.14
90	CG	ASP	A	823	-22.349	-4.965	24.976	1.00	41.63
91	OD1	ASP	A	823	-23.018	-4.67	25.991	1.00	41.35
92	OD2	ASP	A	823	-22.868	-5.185	23.861	1.00	42.15
93	N	ILE	A	824	-17.826	-3.55	25.883	1.00	37.96
94	CA	ILE	A	824	-16.431	-3.832	26.196	1.00	37.49
95	C	ILE	A	824	-15.922	-3.025	27.384	1.00	37.91
96	O	ILE	A	824	-16.046	-1.805	27.42	1.00	38.26
97	CB	ILE	A	824	-15.531	-3.541	24.989	1.00	36.24
98	CG1	ILE	A	824	-15.999	-4.378	23.796	1.00	35.14
99	CG2	ILE	A	824	-14.072	-3.815	25.351	1.00	35.25
100	CD1	ILE	A	824	-15.291	-4.064	22.506	1.00	34.5
101	N	LYS	A	825	-15.348	-3.719	28.357	1.00	38.78
102	CA	LYS	A	825	-14.809	-3.069	29.54	1.00	39.64
103	C	LYS	A	825	-13.325	-3.407	29.628	1.00	38.89
104	O	LYS	A	825	-12.958	-4.566	29.8	1.00	39.22
105	CB	LYS	A	825	-15.546	-3.571	30.782	1.00	41.79
106	CG	LYS	A	825	-15.161	-2.883	32.083	1.00	45.99
107	CD	LYS	A	825	-16.02	-3.415	33.225	1.00	49.18
108	CE	LYS	A	825	-15.823	-2.632	34.511	1.00	50.73
109	NZ	LYS	A	825	-16.776	-3.082	35.57	1.00	51.28
110	N	PHE	A	826	-12.473	-2.397	29.487	1.00	38.04
111	CA	PHE	A	826	-11.03	-2.606	29.552	1.00	37.43
112	C	PHE	A	826	-10.58	-2.636	31.003	1.00	36.81
113	O	PHE	A	826	-11.021	-1.821	31.807	1.00	37.15
114	CB	PHE	A	826	-10.307	-1.489	28.804	1.00	37.41
115	CG	PHE	A	826	-10.74	-1.35	27.377	1.00	37.08
116	CD1	PHE	A	826	-11.5	-0.262	26.971	1.00	36.89

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TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

117	CD2	PHE	A	826	-10.401	-2.322	26.439	1.00	36.86
118	CE1	PHE	A	826	-11.917	-0.145	25.653	1.00	37.26
119	CE2	PHE	A	826	-10.812	-2.214	25.122	1.00	36.03
120	CZ	PHE	A	826	-11.571	-1.125	24.725	1.00	37.36
121	N	GLN	A	827	-9.693	-3.565	31.341	1.00	35.69
122	CA	GLN	A	827	-9.239	-3.677	32.721	1.00	36.08
123	C	GLN	A	827	-7.735	-3.525	32.927	1.00	35.26
124	O	GLN	A	827	-7.302	-3.042	33.967	1.00	34.07
125	CB	GLN	A	827	-9.683	-5.021	33.305	1.00	37.12
126	CG	GLN	A	827	-11.088	-5.443	32.901	1.00	39.59
127	CD	GLN	A	827	-11.425	-6.85	33.361	1.00	41.25
128	OE1	GLN	A	827	-11.803	-7.069	34.511	1.00	41.89
129	NE2	GLN	A	827	-11.276	-7.815	32.463	1.00	41.67
130	N	ASP	A	828	-6.937	-3.927	31.944	1.00	35.07
131	CA	ASP	A	828	-5.49	-3.847	32.098	1.00	34.84
132	C	ASP	A	828	-4.803	-4.01	30.748	1.00	34.59
133	O	ASP	A	828	-5.452	-4.23	29.724	1.00	34.52
134	CB	ASP	A	828	-5.032	-4.968	33.04	1.00	36.76
135	CG	ASP	A	828	-3.681	-4.7	33.69	1.00	37.34
136	OD1	ASP	A	828	-2.911	-3.85	33.2	1.00	38.22
137	OD2	ASP	A	828	-3.387	-5.37	34.702	1.00	38.31
138	N	VAL	A	829	-3.482	-3.881	30.76	1.00	34.07
139	CA	VAL	A	829	-2.669	-4.055	29.565	1.00	33.59
140	C	VAL	A	829	-1.726	-5.204	29.892	1.00	32.05
141	O	VAL	A	829	-1.075	-5.199	30.937	1.00	31.47
142	CB	VAL	A	829	-1.838	-2.791	29.238	1.00	34.25
143	CG1	VAL	A	829	-0.791	-3.106	28.181	1.00	33.31
144	CG2	VAL	A	829	-2.758	-1.687	28.736	1.00	36.5
145	N	ILE	A	830	-1.671	-6.193	29.007	1.00	30.75
146	CA	ILE	A	830	-0.817	-7.358	29.21	1.00	30.2
147	C	ILE	A	830	-0.225	-7.818	27.886	1.00	30.4
148	O	ILE	A	830	-0.519	-7.254	26.832	1.00	32.98
149	CB	ILE	A	830	-1.611	-8.542	29.792	1.00	29.02
150	CG1	ILE	A	830	-2.692	-8.965	28.797	1.00	29.6
151	CG2	ILE	A	830	-2.237	-8.163	31.134	1.00	27.58
152	CD1	ILE	A	830	-3.38	-10.26	29.167	1.00	30.24
153	N	GLY	A	831	0.617	-8.844	27.946	1.00	29.67
154	CA	GLY	A	831	1.215	-9.385	26.74	1.00	27.5
155	C	GLY	A	831	0.574	-10.732	26.457	1.00	26.98

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

156	O	GLY	A	831	0.07	-11.381	27.371	1.00	25.77
157	N	GLU	A	832	0.569	-11.154	25.198	1.00	26.42
158	CA	GLU	A	832	-0.019	-12.44	24.848	1.00	25.78
159	C	GLU	A	832	0.657	-13.057	23.627	1.00	24.99
160	O	GLU	A	832	0.113	-13.028	22.526	1.00	24.4
161	CB	GLU	A	832	-1.525	-12.291	24.592	1.00	24.68
162	CG	GLU	A	832	-2.226	-13.633	24.431	1.00	25.53
163	CD	GLU	A	832	-3.725	-13.554	24.61	1.00	26.04
164	OE1	GLU	A	832	-4.199	-12.636	25.311	1.00	25.36
165	OE2	GLU	A	832	-4.431	-14.43	24.07	1.00	26.49
166	N	GLY	A	833	1.846	-13.618	23.836	1.00	24.85
167	CA	GLY	A	833	2.579	-14.238	22.749	1.00	22.75
168	C	GLY	A	833	2.847	-13.263	21.624	1.00	22.85
169	O	GLY	A	833	3.123	-12.085	21.872	1.00	21.63
170	N	ASN	A	834	2.75	-13.739	20.385	1.00	21.42
171	CA	ASN	A	834	2.997	-12.88	19.234	1.00	22.26
172	C	ASN	A	834	1.913	-11.831	18.976	1.00	21.84
173	O	ASN	A	834	1.98	-11.101	17.987	1.00	22.2
174	CB	ASN	A	834	3.251	-13.723	17.98	1.00	21.15
175	CG	ASN	A	834	2.201	-14.79	17.771	1.00	23.02
176	OD1	ASN	A	834	2.458	-15.807	17.121	1.00	24.64
177	ND2	ASN	A	834	1.01	-14.567	18.309	1.00	19.77
178	N	PHE	A	835	0.913	-11.758	19.852	1.00	21.09
179	CA	PHE	A	835	-0.116	-10.732	19.709	1.00	23.61
180	C	PHE	A	835	0.485	-9.433	20.243	1.00	24.55
181	O	PHE	A	835	-0.054	-8.345	20.026	1.00	26.16
182	CB	PHE	A	835	-1.37	-11.042	20.54	1.00	22.85
183	CG	PHE	A	835	-2.319	-12.007	19.887	1.00	24.42
184	CD1	PHE	A	835	-2.241	-13.371	20.154	1.00	24.05
185	CD2	PHE	A	835	-3.307	-11.547	19.02	1.00	23.02
186	CE1	PHE	A	835	-3.138	-14.267	19.567	1.00	25.04
187	CE2	PHE	A	835	-4.207	-12.429	18.427	1.00	24.58
188	CZ	PHE	A	835	-4.125	-13.794	18.701	1.00	24.72
189	N	GLY	A	836	1.606	-9.557	20.947	1.00	24.91
190	CA	GLY	A	836	2.237	-8.389	21.529	1.00	25.15
191	C	GLY	A	836	1.395	-7.921	22.704	1.00	26.01
192	O	GLY	A	836	0.798	-8.736	23.416	1.00	24.31
193	N	GLN	A	837	1.333	-6.611	22.906	1.00	26.33
194	CA	GLN	A	837	0.558	-6.054	24.005	1.00	29.04

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

195	C	GLN	A	837	-0.928	-6.064	23.682	1.00	27.8
196	O	GLN	A	837	-1.331	-5.679	22.59	1.00	27.62
197	CB	GLN	A	837	1.02	-4.624	24.281	1.00	33.02
198	CG	GLN	A	837	2.476	-4.55	24.707	1.00	38.77
199	CD	GLN	A	837	2.668	-4.933	26.162	1.00	42.1
200	OE1	GLN	A	837	2.559	-4.088	27.053	1.00	44.18
201	NE2	GLN	A	837	2.938	-6.212	26.413	1.00	43.17
202	N	VAL	A	838	-1.739	-6.519	24.631	1.00	26.03
203	CA	VAL	A	838	-3.18	-6.561	24.435	1.00	24.5
204	C	VAL	A	838	-3.904	-6.034	25.663	1.00	25.38
205	O	VAL	A	838	-3.337	-5.948	26.75	1.00	22.99
206	CB	VAL	A	838	-3.686	-7.998	24.139	1.00	24.99
207	CG1	VAL	A	838	-3.181	-8.457	22.78	1.00	22.87
208	CG2	VAL	A	838	-3.23	-8.958	25.241	1.00	23.63
209	N	LEU	A	839	-5.173	-5.693	25.487	1.00	26.33
210	CA	LEU	A	839	-5.962	-5.168	26.585	1.00	27.51
211	C	LEU	A	839	-6.78	-6.263	27.266	1.00	28.97
212	O	LEU	A	839	-7.632	-6.888	26.635	1.00	28.95
213	CB	LEU	A	839	-6.894	-4.072	26.059	1.00	27.52
214	CG	LEU	A	839	-6.208	-2.805	25.539	1.00	27.66
215	CD1	LEU	A	839	-7.056	-2.145	24.472	1.00	28.78
216	CD2	LEU	A	839	-5.969	-1.858	26.694	1.00	28.87
217	N	LYS	A	840	-6.51	-6.511	28.544	1.00	29.74
218	CA	LYS	A	840	-7.289	-7.499	29.278	1.00	31.69
219	C	LYS	A	840	-8.65	-6.838	29.434	1.00	32.56
220	O	LYS	A	840	-8.739	-5.709	29.923	1.00	33.11
221	CB	LYS	A	840	-6.69	-7.766	30.661	1.00	33.16
222	CG	LYS	A	840	-7.517	-8.735	31.514	1.00	34.98
223	CD	LYS	A	840	-6.781	-9.127	32.791	1.00	37.42
224	CE	LYS	A	840	-7.591	-10.099	33.646	1.00	39.15
225	NZ	LYS	A	840	-8.85	-9.501	34.181	1.00	40.38
226	N	ALA	A	841	-9.705	-7.523	29.018	1.00	32.13
227	CA	ALA	A	841	-11.034	-6.94	29.108	1.00	31.73
228	C	ALA	A	841	-12.137	-7.934	29.441	1.00	31.87
229	O	ALA	A	841	-11.892	-9.113	29.688	1.00	31.11
230	CB	ALA	A	841	-11.362	-6.24	27.798	1.00	31
231	N	ARG	A	842	-13.357	-7.414	29.466	1.00	32.15
232	CA	ARG	A	842	-14.553	-8.196	29.716	1.00	33.28
233	C	ARG	A	842	-15.495	-7.802	28.592	1.00	32.99

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234	O	ARG	A	842	-15.74	-6.618	28.366	1.00	32.56
235	CB	ARG	A	842	-15.186	-7.837	31.062	1.00	34.6
236	CG	ARG	A	842	-14.402	-8.295	32.274	1.00	37.39
237	CD	ARG	A	842	-15.337	-8.957	33.273	1.00	40.41
238	NE	ARG	A	842	-15.313	-10.411	33.156	1.00	43.75
239	CZ	ARG	A	842	-16.291	-11.216	33.559	1.00	45.24
240	NH1	ARG	A	842	-17.391	-10.713	34.107	1.00	45.18
241	NH2	ARG	A	842	-16.162	-12.531	33.422	1.00	46.94
242	N	ILE	A	843	-16.008	-8.792	27.876	1.00	33.91
243	CA	ILE	A	843	-16.909	-8.526	26.766	1.00	34.53
244	C	ILE	A	843	-18.204	-9.286	26.969	1.00	35.76
245	O	ILE	A	843	-18.333	-10.082	27.901	1.00	35.28
246	CB	ILE	A	843	-16.293	-8.978	25.417	1.00	34.31
247	CG1	ILE	A	843	-16.133	-10.506	25.404	1.00	34.49
248	CG2	ILE	A	843	-14.942	-8.3	25.207	1.00	33.54
249	CD1	ILE	A	843	-15.606	-11.075	24.086	1.00	33.99
250	N	LYS	A	844	-19.164	-9.033	26.09	1.00	37.38
251	CA	LYS	A	844	-20.436	-9.724	26.154	1.00	38.94
252	C	LYS	A	844	-20.493	-10.644	24.948	1.00	40.14
253	O	LYS	A	844	-20.24	-10.217	23.82	1.00	40.3
254	CB	LYS	A	844	-21.602	-8.735	26.112	1.00	40.07
255	CG	LYS	A	844	-22.948	-9.378	26.423	1.00	43.14
256	CD	LYS	A	844	-24.082	-8.357	26.441	1.00	45.48
257	CE	LYS	A	844	-25.379	-8.995	26.923	1.00	47.1
258	NZ	LYS	A	844	-26.518	-8.03	27.015	1.00	48.65
259	N	LYS	A	845	-20.796	-11.914	25.189	1.00	40.83
260	CA	LYS	A	845	-20.906	-12.881	24.111	1.00	42.22
261	C	LYS	A	845	-21.947	-13.93	24.474	1.00	42.55
262	O	LYS	A	845	-21.91	-14.51	25.562	1.00	41.69
263	CB	LYS	A	845	-19.558	-13.547	23.84	1.00	43.94
264	CG	LYS	A	845	-19.568	-14.432	22.61	1.00	46.03
265	CD	LYS	A	845	-18.185	-14.976	22.291	1.00	48.74
266	CE	LYS	A	845	-18.215	-15.777	21	1.00	50.01
267	NZ	LYS	A	845	-16.871	-16.286	20.628	1.00	52.56
268	N	ASP	A	846	-22.877	-14.16	23.552	1.00	43.37
269	CA	ASP	A	846	-23.955	-15.119	23.754	1.00	42.7
270	C	ASP	A	846	-24.738	-14.751	25.012	1.00	41.58
271	O	ASP	A	846	-25.124	-15.616	25.794	1.00	40.92
272	CB	ASP	A	846	-23.391	-16.543	23.869	1.00	44.87

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

273	CG	ASP	A	846	-22.589	-16.953	22.639	1.00	46.22
274	OD1	ASP	A	846	-23.072	-16.716	21.511	1.00	46.71
275	OD2	ASP	A	846	-21.484	-17.518	22.799	1.00	47.12
276	N	GLY	A	847	-24.949	-13.449	25.198	1.00	40.32
277	CA	GLY	A	847	-25.69	-12.954	26.344	1.00	39.2
278	C	GLY	A	847	-24.957	-12.963	27.674	1.00	38.73
279	O	GLY	A	847	-25.501	-12.518	28.68	1.00	38.75
280	N	LEU	A	848	-23.724	-13.454	27.693	1.00	38.22
281	CA	LEU	A	848	-22.971	-13.51	28.938	1.00	38.28
282	C	LEU	A	848	-21.704	-12.659	28.94	1.00	38.59
283	O	LEU	A	848	-21.053	-12.473	27.91	1.00	38.46
284	CB	LEU	A	848	-22.603	-14.962	29.251	1.00	37.66
285	CG	LEU	A	848	-23.776	-15.944	29.335	1.00	39.01
286	CD1	LEU	A	848	-23.253	-17.365	29.428	1.00	39.07
287	CD2	LEU	A	848	-24.644	-15.608	30.537	1.00	38.7
288	N	ARG	A	849	-21.363	-12.145	30.116	1.00	38.74
289	CA	ARG	A	849	-20.168	-11.336	30.298	1.00	38.64
290	C	ARG	A	849	-19.032	-12.318	30.571	1.00	37.93
291	O	ARG	A	849	-19.152	-13.173	31.445	1.00	37.33
292	CB	ARG	A	849	-20.351	-10.405	31.497	1.00	39.46
293	CG	ARG	A	849	-21.543	-9.472	31.383	1.00	41.57
294	CD	ARG	A	849	-21.264	-8.372	30.393	1.00	43
295	NE	ARG	A	849	-20.16	-7.531	30.843	1.00	45.35
296	CZ	ARG	A	849	-19.526	-6.666	30.062	1.00	46.3
297	NH1	ARG	A	849	-18.53	-5.935	30.543	1.00	47.59
298	NH2	ARG	A	849	-19.888	-6.542	28.796	1.00	46.78
299	N	MET	A	850	-17.939	-12.198	29.822	1.00	36.96
300	CA	MET	A	850	-16.802	-13.094	29.987	1.00	35.76
301	C	MET	A	850	-15.465	-12.378	29.852	1.00	34.62
302	O	MET	A	850	-15.395	-11.246	29.379	1.00	34.72
303	CB	MET	A	850	-16.854	-14.213	28.947	1.00	37.6
304	CG	MET	A	850	-16.661	-13.725	27.514	1.00	39.7
305	SD	MET	A	850	-16.328	-15.065	26.351	1.00	43.49
306	CE	MET	A	850	-17.977	-15.535	25.872	1.00	44.23
307	N	ASP	A	851	-14.404	-13.062	30.264	1.00	32.53
308	CA	ASP	A	851	-13.056	-12.528	30.179	1.00	31.78
309	C	ASP	A	851	-12.558	-12.651	28.744	1.00	29.68
310	O	ASP	A	851	-12.945	-13.563	28.013	1.00	29.52
311	CB	ASP	A	851	-12.111	-13.318	31.093	1.00	33.54

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312	CG	ASP	A	851	-12.337	-13.034	32.561	1.00	35.36
313	OD1	ASP	A	851	-12.103	-13.953	33.369	1.00	36.96
314	OD2	ASP	A	851	-12.731	-11.9	32.912	1.00	35.51
315	N	ALA	A	852	-11.694	-11.731	28.346	1.00	27.41
316	CA	ALA	A	852	-11.113	-11.76	27.016	1.00	26.29
317	C	ALA	A	852	-9.963	-10.776	26.976	1.00	26.19
318	O	ALA	A	852	-9.723	-10.041	27.934	1.00	26.53
319	CB	ALA	A	852	-12.15	-11.393	25.966	1.00	25.47
320	N	ALA	A	853	-9.234	-10.786	25.871	1.00	24.98
321	CA	ALA	A	853	-8.133	-9.864	25.693	1.00	24.58
322	C	ALA	A	853	-8.432	-9.188	24.373	1.00	24.91
323	O	ALA	A	853	-9.043	-9.788	23.491	1.00	24.78
324	CB	ALA	A	853	-6.812	-10.611	25.632	1.00	23.92
325	N	ILE	A	854	-8.025	-7.936	24.233	1.00	25.16
326	CA	ILE	A	854	-8.293	-7.234	22.998	1.00	26.27
327	C	ILE	A	854	-7.045	-6.677	22.34	1.00	26.38
328	O	ILE	A	854	-6.261	-5.958	22.957	1.00	26.11
329	CB	ILE	A	854	-9.321	-6.101	23.219	1.00	27.54
330	CG1	ILE	A	854	-10.665	-6.715	23.628	1.00	27.93
331	CG2	ILE	A	854	-9.476	-5.273	21.948	1.00	27.1
332	CD1	ILE	A	854	-11.795	-5.723	23.74	1.00	30.46
333	N	LYS	A	855	-6.873	-7.051	21.078	1.00	26.73
334	CA	LYS	A	855	-5.753	-6.613	20.264	1.00	28.02
335	C	LYS	A	855	-6.264	-5.465	19.403	1.00	28.89
336	O	LYS	A	855	-7.183	-5.639	18.611	1.00	28.27
337	CB	LYS	A	855	-5.273	-7.772	19.378	1.00	28.1
338	CG	LYS	A	855	-4.232	-7.409	18.323	1.00	28.97
339	CD	LYS	A	855	-2.941	-6.893	18.942	1.00	27.87
340	CE	LYS	A	855	-1.879	-6.672	17.876	1.00	27.67
341	NZ	LYS	A	855	-0.642	-6.053	18.42	1.00	28.38
342	N	ARG	A	856	-5.675	-4.288	19.575	1.00	30.61
343	CA	ARG	A	856	-6.067	-3.119	18.807	1.00	32.86
344	C	ARG	A	856	-5.226	-3.051	17.533	1.00	34.26
345	O	ARG	A	856	-3.994	-3.027	17.585	1.00	33.81
346	CB	ARG	A	856	-5.86	-1.86	19.648	1.00	34.28
347	CG	ARG	A	856	-6.69	-0.673	19.214	1.00	37.26
348	CD	ARG	A	856	-6.566	0.454	20.215	1.00	38.28
349	NE	ARG	A	856	-5.298	1.153	20.079	1.00	41.05
350	CZ	ARG	A	856	-5.16	2.327	19.473	1.00	41.18



TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

351	NH1	ARG	A	856	-6.218	2.933	18.952	1.00	41.18
352	NH2	ARG	A	856	-3.963	2.889	19.387	1.00	40.84
353	N	MET	A	857	-5.901	-3.031	16.387	1.00	36.18
354	CA	MET	A	857	-5.226	-2.978	15.095	1.00	38.28
355	C	MET	A	857	-5.582	-1.703	14.335	1.00	40.13
356	O	MET	A	857	-6.756	-1.415	14.097	1.00	39.53
357	CB	MET	A	857	-5.61	-4.204	14.256	1.00	37.64
358	CG	MET	A	857	-5.127	-5.53	14.83	1.00	38.3
359	SD	MET	A	857	-5.827	-6.997	14.025	1.00	38.71
360	CE	MET	A	857	-4.904	-7.006	12.488	1.00	37.94
361	N	ALA	A	858	-4.566	-0.931	13.967	1.00	42.66
362	CA	ALA	A	858	-4.793	0.298	13.217	1.00	45.71
363	C	ALA	A	858	-5.157	-0.119	11.799	1.00	47.45
364	O	ALA	A	858	-4.431	-0.886	11.164	1.00	47.49
365	CB	ALA	A	858	-3.53	1.167	13.215	1.00	46.11
366	N	GLU	A	859	-6.286	0.375	11.308	1.00	49.54
367	CA	GLU	A	859	-6.732	0.019	9.974	1.00	52.67
368	C	GLU	A	859	-6.03	0.807	8.874	1.00	54.55
369	O	GLU	A	859	-5.979	0.364	7.726	1.00	55.16
370	CB	GLU	A	859	-8.247	0.194	9.881	1.00	53.29
371	CG	GLU	A	859	-8.997	-0.742	10.811	1.00	55.14
372	CD	GLU	A	859	-10.5	-0.629	10.686	1.00	56.3
373	OE1	GLU	A	859	-11.048	0.447	11.009	1.00	56.82
374	OE2	GLU	A	859	-11.133	-1.62	10.266	1.00	57.51
375	N	ALA	A	860	-5.476	1.963	9.226	1.00	56.04
376	CA	ALA	A	860	-4.774	2.797	8.254	1.00	58.16
377	CB	ALA	A	860	-4.929	4.273	8.622	1.00	58.04
378	C	ALA	A	860	-3.291	2.424	8.183	1.00	59.13
379	OT1	ALA	A	860	-2.443	3.333	8.328	1.00	59.46
380	OT2	ALA	A	860	-2.996	1.225	7.98	1.00	59.83
381	N	ALA	A	867	-3.168	-3.892	1.676	1.00	67.16
382	CA	ALA	A	867	-2.469	-3.202	2.797	1.00	66.6
383	C	ALA	A	867	-1.868	-4.213	3.769	1.00	66.18
384	O	ALA	A	867	-2.119	-5.417	3.67	1.00	65.81
385	CB	ALA	A	867	-3.444	-2.286	3.538	1.00	66.64
386	N	ASP	A	868	-1.072	-3.71	4.707	1.00	65.27
387	CA	ASP	A	868	-0.43	-4.546	5.714	1.00	64.08
388	C	ASP	A	868	-1.49	-5.081	6.685	1.00	62.72
389	O	ASP	A	868	-1.359	-6.183	7.222	1.00	62.05

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

390	CB	ASP	A	868	0.61	-3.719	6.473	1.00	65.69
391	CG	ASP	A	868	1.548	-4.572	7.3	1.00	66.89
392	OD1	ASP	A	868	1.059	-5.337	8.159	1.00	68.35
393	OD2	ASP	A	868	2.777	-4.473	7.091	1.00	67.45
394	N	PHE	A	869	-2.539	-4.285	6.892	1.00	60.74
395	CA	PHE	A	869	-3.645	-4.633	7.783	1.00	58.16
396	C	PHE	A	869	-4.548	-5.703	7.176	1.00	56.63
397	O	PHE	A	869	-4.849	-6.711	7.814	1.00	56.02
398	CB	PHE	A	869	-4.481	-3.384	8.084	1.00	57.94
399	CG	PHE	A	869	-5.779	-3.673	8.785	1.00	57.81
400	CD1	PHE	A	869	-5.795	-4.055	10.123	1.00	57.93
401	CD2	PHE	A	869	-6.988	-3.572	8.102	1.00	57.33
402	CE1	PHE	A	869	-6.999	-4.333	10.772	1.00	57.2
403	CE2	PHE	A	869	-8.195	-3.848	8.741	1.00	57.07
404	CZ	PHE	A	869	-8.201	-4.228	10.079	1.00	57.13
405	N	ALA	A	870	-4.988	-5.465	5.946	1.00	55.24
406	CA	ALA	A	870	-5.859	-6.401	5.247	1.00	53.46
407	C	ALA	A	870	-5.184	-7.759	5.112	1.00	52.41
408	O	ALA	A	870	-5.851	-8.791	5.075	1.00	52.04
409	CB	ALA	A	870	-6.213	-5.854	3.873	1.00	53.03
410	N	GLY	A	871	-3.857	-7.746	5.036	1.00	50.91
411	CA	GLY	A	871	-3.106	-8.98	4.907	1.00	49.32
412	C	GLY	A	871	-3.212	-9.87	6.13	1.00	48.3
413	O	GLY	A	871	-3.596	-11.035	6.026	1.00	47.15
414	N	GLU	A	872	-2.879	-9.329	7.297	1.00	47.41
415	CA	GLU	A	872	-2.944	-10.114	8.519	1.00	47.39
416	C	GLU	A	872	-4.376	-10.416	8.953	1.00	46.13
417	O	GLU	A	872	-4.611	-11.315	9.759	1.00	46.19
418	CB	GLU	A	872	-2.164	-9.415	9.638	1.00	48.67
419	CG	GLU	A	872	-2.597	-8.003	9.961	1.00	51.45
420	CD	GLU	A	872	-1.503	-7.217	10.669	1.00	52.87
421	OE1	GLU	A	872	-0.695	-7.837	11.39	1.00	53.97
422	OE2	GLU	A	872	-1.456	-5.98	10.513	1.00	53.82
423	N	LEU	A	873	-5.335	-9.682	8.4	1.00	45.17
424	CA	LEU	A	873	-6.738	-9.901	8.727	1.00	44.42
425	C	LEU	A	873	-7.259	-11.094	7.925	1.00	43.93
426	O	LEU	A	873	-8.109	-11.855	8.392	1.00	43.63
427	CB	LEU	A	873	-7.56	-8.655	8.394	1.00	45.09
428	CG	LEU	A	873	-9.027	-8.69	8.825	1.00	45.6

TABLE 2  
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429	CD1	LEU	A	873	-9.106	-8.737	10.349	1.00	46.02
430	CD2	LEU	A	873	-9.748	-7.462	8.29	1.00	45.68
431	N	GLU	A	874	-6.739	-11.254	6.712	1.00	43.71
432	CA	GLU	A	874	-7.144	-12.358	5.854	1.00	43.72
433	C	GLU	A	874	-6.632	-13.665	6.44	1.00	41.9
434	O	GLU	A	874	-7.298	-14.698	6.364	1.00	40.53
435	CB	GLU	A	874	-6.586	-12.181	4.441	1.00	46.48
436	CG	GLU	A	874	-6.955	-13.32	3.504	1.00	51.23
437	CD	GLU	A	874	-6.337	-13.175	2.128	1.00	54.51
438	OE1	GLU	A	874	-6.629	-12.169	1.441	1.00	55.89
439	OE2	GLU	A	874	-5.559	-14.072	1.731	1.00	56.63
440	N	VAL	A	875	-5.437	-13.618	7.021	1.00	40.04
441	CA	VAL	A	875	-4.862	-14.808	7.628	1.00	37.75
442	C	VAL	A	875	-5.659	-15.158	8.884	1.00	36.31
443	O	VAL	A	875	-6.039	-16.306	9.078	1.00	34.93
444	CB	VAL	A	875	-3.372	-14.594	7.999	1.00	38.03
445	CG1	VAL	A	875	-2.817	-15.852	8.658	1.00	36.56
446	CG2	VAL	A	875	-2.565	-14.252	6.746	1.00	36.06
447	N	LEU	A	876	-5.926	-14.163	9.725	1.00	35.51
448	CA	LEU	A	876	-6.684	-14.393	10.953	1.00	35.89
449	C	LEU	A	876	-8.05	-15.037	10.712	1.00	36.49
450	O	LEU	A	876	-8.546	-15.78	11.559	1.00	36
451	CB	LEU	A	876	-6.864	-13.081	11.722	1.00	35.2
452	CG	LEU	A	876	-5.608	-12.508	12.383	1.00	34.83
453	CD1	LEU	A	876	-5.907	-11.129	12.957	1.00	34.14
454	CD2	LEU	A	876	-5.125	-13.461	13.476	1.00	34.24
455	N	CYS	A	877	-8.653	-14.756	9.559	1.00	37.59
456	CA	CYS	A	877	-9.961	-15.317	9.224	1.00	39.35
457	C	CYS	A	877	-9.896	-16.765	8.746	1.00	38.57
458	O	CYS	A	877	-10.92	-17.44	8.649	1.00	38.76
459	CB	CYS	A	877	-10.652	-14.464	8.156	1.00	41.84
460	SG	CYS	A	877	-11.342	-12.918	8.785	1.00	48.61
461	N	LYS	A	878	-8.695	-17.237	8.443	1.00	37.51
462	CA	LYS	A	878	-8.508	-18.604	7.986	1.00	37.07
463	C	LYS	A	878	-8.185	-19.507	9.173	1.00	36.78
464	O	LYS	A	878	-8.027	-20.718	9.015	1.00	36.69
465	CB	LYS	A	878	-7.353	-18.676	6.985	1.00	38.29
466	CG	LYS	A	878	-7.505	-17.797	5.752	1.00	39.91
467	CD	LYS	A	878	-8.668	-18.232	4.878	1.00	42.79

TABLE 2  
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468	CE	LYS	A	878	-8.703	-17.424	3.58	1.00	44.91
469	NZ	LYS	A	878	-9.848	-17.813	2.714	1.00	46.64
470	N	LEU	A	879	-8.081	-18.917	10.359	1.00	35.63
471	CA	LEU	A	879	-7.742	-19.694	11.543	1.00	35.03
472	C	LEU	A	879	-8.788	-20.726	11.932	1.00	34.67
473	O	LEU	A	879	-8.453	-21.867	12.239	1.00	34.78
474	CB	LEU	A	879	-7.471	-18.767	12.735	1.00	34.6
475	CG	LEU	A	879	-6.155	-17.98	12.75	1.00	32.75
476	CD1	LEU	A	879	-6.097	-17.12	13.999	1.00	33.12
477	CD2	LEU	A	879	-4.979	-18.938	12.714	1.00	32.58
478	N	GLY	A	880	-10.054	-20.335	11.916	1.00	33.87
479	CA	GLY	A	880	-11.092	-21.266	12.31	1.00	33.95
480	C	GLY	A	880	-11.039	-21.423	13.82	1.00	34.06
481	O	GLY	A	880	-10.63	-20.502	14.525	1.00	34.7
482	N	HIS	A	881	-11.438	-22.585	14.324	1.00	33.37
483	CA	HIS	A	881	-11.415	-22.823	15.76	1.00	33.33
484	C	HIS	A	881	-10.786	-24.162	16.128	1.00	31.88
485	O	HIS	A	881	-10.913	-25.147	15.401	1.00	31.25
486	CB	HIS	A	881	-12.835	-22.745	16.336	1.00	35
487	CG	HIS	A	881	-13.372	-21.35	16.412	1.00	39.19
488	ND1	HIS	A	881	-12.927	-20.432	17.339	1.00	41.28
489	CD2	HIS	A	881	-14.285	-20.702	15.65	1.00	41
490	CE1	HIS	A	881	-13.543	-19.279	17.145	1.00	41.61
491	NE2	HIS	A	881	-14.371	-19.416	16.125	1.00	41.86
492	N	HIS	A	882	-10.088	-24.167	17.26	1.00	28.7
493	CA	HIS	A	882	-9.445	-25.363	17.782	1.00	27.06
494	C	HIS	A	882	-9.079	-25.091	19.227	1.00	24.88
495	O	HIS	A	882	-8.641	-23.997	19.569	1.00	25.27
496	CB	HIS	A	882	-8.192	-25.733	16.984	1.00	26.04
497	CG	HIS	A	882	-7.622	-27.063	17.363	1.00	27.59
498	ND1	HIS	A	882	-6.818	-27.244	18.472	1.00	27.59
499	CD2	HIS	A	882	-7.794	-28.293	16.821	1.00	27.89
500	CE1	HIS	A	882	-6.525	-28.527	18.594	1.00	27.2
501	NE2	HIS	A	882	-7.105	-29.184	17.608	1.00	27.24
502	N	PRO	A	883	-9.26	-26.086	20.099	1.00	24.5
503	CA	PRO	A	883	-8.948	-25.929	21.52	1.00	24.29
504	C	PRO	A	883	-7.507	-25.541	21.822	1.00	23
505	O	PRO	A	883	-7.246	-24.875	22.816	1.00	21.33
506	CB	PRO	A	883	-9.299	-27.297	22.109	1.00	24.81

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507	CG	PRO	A	883	-10.356	-27.813	21.183	1.00	25.72
508	CD	PRO	A	883	-9.81	-27.425	19.829	1.00	24.65
509	N	ASN	A	884	-6.576	-25.944	20.966	1.00	21.88
510	CA	ASN	A	884	-5.175	-25.652	21.234	1.00	21.08
511	C	ASN	A	884	-4.56	-24.438	20.543	1.00	20.76
512	O	ASN	A	884	-3.34	-24.363	20.387	1.00	18.95
513	CB	ASN	A	884	-4.34	-26.911	20.98	1.00	19.35
514	CG	ASN	A	884	-4.709	-28.033	21.928	1.00	21.38
515	OD1	ASN	A	884	-5.012	-29.151	21.506	1.00	21.48
516	ND2	ASN	A	884	-4.698	-27.736	23.225	1.00	21.21
517	N	ILE	A	885	-5.405	-23.501	20.113	1.00	19.85
518	CA	ILE	A	885	-4.91	-22.263	19.51	1.00	19.62
519	C	ILE	A	885	-5.652	-21.137	20.216	1.00	20.29
520	O	ILE	A	885	-6.606	-21.39	20.951	1.00	19.69
521	CB	ILE	A	885	-5.189	-22.158	17.988	1.00	18.84
522	CG1	ILE	A	885	-6.697	-22.074	17.728	1.00	20.08
523	CG2	ILE	A	885	-4.555	-23.334	17.252	1.00	18.08
524	CD1	ILE	A	885	-7.044	-21.796	16.28	1.00	19.94
525	N	ILE	A	886	-5.204	-19.9	20.029	1.00	20.53
526	CA	ILE	A	886	-5.897	-18.775	20.641	1.00	19.72
527	C	ILE	A	886	-7.039	-18.492	19.673	1.00	20.51
528	O	ILE	A	886	-6.811	-18.197	18.504	1.00	19.74
529	CB	ILE	A	886	-4.981	-17.529	20.761	1.00	19.34
530	CG1	ILE	A	886	-3.929	-17.757	21.859	1.00	18.39
531	CG2	ILE	A	886	-5.824	-16.277	21.035	1.00	16.1
532	CD1	ILE	A	886	-4.497	-17.91	23.26	1.00	15.63
533	N	ASN	A	887	-8.267	-18.604	20.156	1.00	21.94
534	CA	ASN	A	887	-9.426	-18.385	19.304	1.00	24.3
535	C	ASN	A	887	-9.931	-16.95	19.293	1.00	25.88
536	O	ASN	A	887	-9.814	-16.227	20.28	1.00	26.07
537	CB	ASN	A	887	-10.556	-19.333	19.722	1.00	25.2
538	CG	ASN	A	887	-10.233	-20.787	19.421	1.00	24.65
539	OD1	ASN	A	887	-10.195	-21.202	18.26	1.00	24.43
540	ND2	ASN	A	887	-9.977	-21.564	20.465	1.00	25.46
541	N	LEU	A	888	-10.479	-16.545	18.15	1.00	27.75
542	CA	LEU	A	888	-11.032	-15.21	17.983	1.00	28.6
543	C	LEU	A	888	-12.45	-15.265	18.531	1.00	29.08
544	O	LEU	A	888	-13.204	-16.188	18.218	1.00	29.1
545	CB	LEU	A	888	-11.049	-14.824	16.502	1.00	29.27

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546	CG	LEU	A	888	-9.709	-14.923	15.759	1.00	30.63
547	CD1	LEU	A	888	-9.83	-14.183	14.426	1.00	31.1
548	CD2	LEU	A	888	-8.576	-14.326	16.598	1.00	28.51
549	N	LEU	A	889	-12.813	-14.278	19.341	1.00	29.2
550	CA	LEU	A	889	-14.13	-14.254	19.96	1.00	31.17
551	C	LEU	A	889	-15.092	-13.246	19.342	1.00	33
552	O	LEU	A	889	-16.3	-13.31	19.566	1.00	34.71
553	CB	LEU	A	889	-13.979	-13.986	21.46	1.00	29.96
554	CG	LEU	A	889	-13.136	-15.02	22.228	1.00	31.35
555	CD1	LEU	A	889	-12.988	-14.6	23.689	1.00	30.05
556	CD2	LEU	A	889	-13.802	-16.395	22.137	1.00	30.24
557	N	GLY	A	890	-14.552	-12.325	18.555	1.00	33.89
558	CA	GLY	A	890	-15.372	-11.316	17.918	1.00	34.79
559	C	GLY	A	890	-14.517	-10.106	17.609	1.00	36.04
560	O	GLY	A	890	-13.314	-10.109	17.877	1.00	35.23
561	N	ALA	A	891	-15.129	-9.07	17.047	1.00	37.23
562	CA	ALA	A	891	-14.393	-7.858	16.708	1.00	39.03
563	C	ALA	A	891	-15.306	-6.639	16.685	1.00	40.17
564	O	ALA	A	891	-16.509	-6.753	16.434	1.00	40.55
565	CB	ALA	A	891	-13.703	-8.024	15.356	1.00	37.17
566	N	CYS	A	892	-14.716	-5.476	16.943	1.00	41.2
567	CA	CYS	A	892	-15.439	-4.214	16.973	1.00	42.18
568	C	CYS	A	892	-14.587	-3.08	16.406	1.00	42.65
569	O	CYS	A	892	-13.465	-2.857	16.86	1.00	41.71
570	CB	CYS	A	892	-15.839	-3.89	18.415	1.00	42.54
571	SG	CYS	A	892	-16.402	-2.195	18.686	1.00	44.31
572	N	GLU	A	893	-15.119	-2.376	15.408	1.00	44.55
573	CA	GLU	A	893	-14.413	-1.251	14.795	1.00	46.52
574	C	GLU	A	893	-14.789	0.016	15.551	1.00	45.98
575	O	GLU	A	893	-15.967	0.28	15.785	1.00	45.81
576	CB	GLU	A	893	-14.793	-1.102	13.318	1.00	49.22
577	CG	GLU	A	893	-14.408	-2.295	12.457	1.00	54.48
578	CD	GLU	A	893	-14.69	-2.072	10.979	1.00	57.06
579	OE1	GLU	A	893	-15.85	-1.756	10.634	1.00	58.97
580	OE2	GLU	A	893	-13.75	-2.217	10.162	1.00	58.32
581	N	HIS	A	894	-13.781	0.796	15.926	1.00	45.88
582	CA	HIS	A	894	-13.995	2.024	16.685	1.00	45.64
583	C	HIS	A	894	-12.946	3.072	16.321	1.00	45.84
584	O	HIS	A	894	-11.746	2.795	16.339	1.00	44.84

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

585	CB	HIS	A	894	-13.912	1.712	18.18	1.00	44.9
586	CG	HIS	A	894	-14.398	2.817	19.063	1.00	44.3
587	ND1	HIS	A	894	-15.731	3.135	19.192	1.00	44.15
588	CD2	HIS	A	894	-13.729	3.654	19.891	1.00	43.93
589	CE1	HIS	A	894	-15.866	4.118	20.063	1.00	43.94
590	NE2	HIS	A	894	-14.666	4.451	20.503	1.00	44.19
591	N	ARG	A	895	-13.415	4.272	15.991	1.00	46.86
592	CA	ARG	A	895	-12.563	5.4	15.618	1.00	46.77
593	C	ARG	A	895	-11.392	5.064	14.698	1.00	45.94
594	O	ARG	A	895	-10.299	5.594	14.875	1.00	46.33
595	CB	ARG	A	895	-12.034	6.1	16.874	1.00	48.59
596	CG	ARG	A	895	-13.128	6.535	17.834	1.00	52.41
597	CD	ARG	A	895	-12.571	7.292	19.032	1.00	56.03
598	NE	ARG	A	895	-12.228	8.674	18.704	1.00	59.85
599	CZ	ARG	A	895	-11.802	9.569	19.592	1.00	62.24
600	NH1	ARG	A	895	-11.517	10.807	19.203	1.00	63.21
601	NH2	ARG	A	895	-11.657	9.228	20.87	1.00	62.96
602	N	GLY	A	896	-11.616	4.188	13.725	1.00	44.71
603	CA	GLY	A	896	-10.557	3.847	12.788	1.00	44.06
604	C	GLY	A	896	-9.658	2.686	13.168	1.00	44.45
605	O	GLY	A	896	-8.697	2.375	12.457	1.00	44.01
606	N	TYR	A	897	-9.965	2.04	14.286	1.00	44.04
607	CA	TYR	A	897	-9.182	0.9	14.754	1.00	43.51
608	C	TYR	A	897	-10.076	-0.33	14.904	1.00	41.79
609	O	TYR	A	897	-11.248	-0.216	15.262	1.00	40.74
610	CB	TYR	A	897	-8.542	1.217	16.111	1.00	44.79
611	CG	TYR	A	897	-7.443	2.256	16.076	1.00	46.65
612	CD1	TYR	A	897	-6.111	1.884	15.895	1.00	47.4
613	CD2	TYR	A	897	-7.733	3.61	16.242	1.00	47.6
614	CE1	TYR	A	897	-5.093	2.836	15.885	1.00	48.35
615	CE2	TYR	A	897	-6.724	4.569	16.232	1.00	48.29
616	CZ	TYR	A	897	-5.407	4.178	16.056	1.00	48.99
617	OH	TYR	A	897	-4.401	5.125	16.065	1.00	50.38
618	N	LEU	A	898	-9.52	-1.502	14.614	1.00	40.41
619	CA	LEU	A	898	-10.26	-2.751	14.758	1.00	37.9
620	C	LEU	A	898	-9.88	-3.366	16.1	1.00	36.35
621	O	LEU	A	898	-8.714	-3.68	16.339	1.00	36.44
622	CB	LEU	A	898	-9.91	-3.736	13.641	1.00	37.14
623	CG	LEU	A	898	-10.564	-5.114	13.797	1.00	37.11

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

624	CD1	LEU	A	898	-12.078	-4.98	13.699	1.00	36.46
625	CD2	LEU	A	898	-10.042	-6.061	12.73	1.00	37.43
626	N	TYR	A	899	-10.862	-3.516	16.98	1.00	34.49
627	CA	TYR	A	899	-10.627	-4.104	18.291	1.00	33.24
628	C	TYR	A	899	-10.981	-5.589	18.229	1.00	32.79
629	O	TYR	A	899	-12.149	-5.964	18.331	1.00	32.99
630	CB	TYR	A	899	-11.472	-3.378	19.339	1.00	32.09
631	CG	TYR	A	899	-10.98	-1.974	19.632	1.00	32
632	CD1	TYR	A	899	-10.196	-1.711	20.756	1.00	31.73
633	CD2	TYR	A	899	-11.249	-0.918	18.755	1.00	31.57
634	CE1	TYR	A	899	-9.69	-0.437	21.002	1.00	31.9
635	CE2	TYR	A	899	-10.742	0.364	18.991	1.00	31.18
636	CZ	TYR	A	899	-9.963	0.597	20.113	1.00	31.48
637	OH	TYR	A	899	-9.431	1.846	20.342	1.00	30.72
638	N	LEU	A	900	-9.956	-6.421	18.052	1.00	31.23
639	CA	LEU	A	900	-10.115	-7.869	17.943	1.00	29.99
640	C	LEU	A	900	-10.1	-8.572	19.306	1.00	28.98
641	O	LEU	A	900	-9.106	-8.526	20.033	1.00	29.08
642	CB	LEU	A	900	-8.997	-8.432	17.055	1.00	30.31
643	CG	LEU	A	900	-8.995	-9.924	16.695	1.00	32.41
644	CD1	LEU	A	900	-10.205	-10.269	15.821	1.00	30.94
645	CD2	LEU	A	900	-7.705	-10.253	15.958	1.00	32.1
646	N	ALA	A	901	-11.209	-9.219	19.65	1.00	27.33
647	CA	ALA	A	901	-11.308	-9.932	20.92	1.00	25.91
648	C	ALA	A	901	-10.797	-11.357	20.745	1.00	24.61
649	O	ALA	A	901	-11.181	-12.052	19.809	1.00	25.14
650	CB	ALA	A	901	-12.76	-9.953	21.408	1.00	24.05
651	N	ILE	A	902	-9.929	-11.786	21.652	1.00	23.33
652	CA	ILE	A	902	-9.37	-13.129	21.597	1.00	23.19
653	C	ILE	A	902	-9.435	-13.791	22.965	1.00	23.17
654	O	ILE	A	902	-9.721	-13.141	23.973	1.00	23.29
655	CB	ILE	A	902	-7.906	-13.098	21.138	1.00	22.47
656	CG1	ILE	A	902	-7.058	-12.335	22.154	1.00	20.47
657	CG2	ILE	A	902	-7.81	-12.443	19.763	1.00	23.12
658	CD1	ILE	A	902	-5.609	-12.257	21.779	1.00	19.9
659	N	GLU	A	903	-9.162	-15.086	23.005	1.00	23.84
660	CA	GLU	A	903	-9.202	-15.799	24.27	1.00	24.9
661	C	GLU	A	903	-8.181	-15.268	25.265	1.00	24.8
662	O	GLU	A	903	-7.032	-14.955	24.917	1.00	24.26



TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

663	CB	GLU	A	903	-8.959	-17.296	24.061	1.00	26.56
664	CG	GLU	A	903	-10.1	-18.035	23.395	1.00	27.97
665	CD	GLU	A	903	-9.833	-19.526	23.313	1.00	28.97
666	OE1	GLU	A	903	-8.826	-19.918	22.689	1.00	28.36
667	OE2	GLU	A	903	-10.628	-20.304	23.88	1.00	31.19
668	N	TYR	A	904	-8.623	-15.171	26.51	1.00	24.29
669	CA	TYR	A	904	-7.784	-14.722	27.601	1.00	25.04
670	C	TYR	A	904	-7.173	-15.962	28.272	1.00	25.28
671	O	TYR	A	904	-7.873	-16.945	28.536	1.00	24.29
672	CB	TYR	A	904	-8.631	-13.925	28.604	1.00	24.94
673	CG	TYR	A	904	-7.945	-13.667	29.923	1.00	25.51
674	CD1	TYR	A	904	-6.755	-12.942	29.983	1.00	26.39
675	CD2	TYR	A	904	-8.472	-14.171	31.11	1.00	26.88
676	CE1	TYR	A	904	-6.105	-12.726	31.192	1.00	27.55
677	CE2	TYR	A	904	-7.829	-13.962	32.328	1.00	27.84
678	CZ	TYR	A	904	-6.644	-13.24	32.362	1.00	28.59
679	OH	TYR	A	904	-5.991	-13.042	33.563	1.00	30.22
680	N	ALA	A	905	-5.867	-15.913	28.523	1.00	25.78
681	CA	ALA	A	905	-5.148	-17.013	29.175	1.00	25.78
682	C	ALA	A	905	-4.839	-16.583	30.609	1.00	26.56
683	O	ALA	A	905	-3.934	-15.782	30.839	1.00	26.99
684	CB	ALA	A	905	-3.856	-17.303	28.423	1.00	25.1
685	N	PRO	A	906	-5.584	-17.115	31.594	1.00	27.47
686	CA	PRO	A	906	-5.383	-16.763	33.01	1.00	27.56
687	C	PRO	A	906	-4.014	-17.11	33.585	1.00	27.96
688	O	PRO	A	906	-3.579	-16.505	34.564	1.00	28.73
689	CB	PRO	A	906	-6.492	-17.536	33.742	1.00	27.3
690	CG	PRO	A	906	-7.466	-17.943	32.655	1.00	28.11
691	CD	PRO	A	906	-6.591	-18.18	31.453	1.00	27.52
692	N	HIS	A	907	-3.331	-18.079	32.985	1.00	27.79
693	CA	HIS	A	907	-2.036	-18.495	33.509	1.00	28.25
694	C	HIS	A	907	-0.79	-17.99	32.771	1.00	28.14
695	O	HIS	A	907	0.312	-18.493	32.992	1.00	29.07
696	CB	HIS	A	907	-2.026	-20.02	33.612	1.00	28.56
697	CG	HIS	A	907	-3.225	-20.571	34.321	1.00	29.49
698	ND1	HIS	A	907	-3.457	-20.357	35.663	1.00	30.18
699	CD2	HIS	A	907	-4.29	-21.27	33.863	1.00	29.9
700	CE1	HIS	A	907	-4.614	-20.9	36.001	1.00	30.21
701	NE2	HIS	A	907	-5.14	-21.46	34.926	1.00	30.57

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

702	N	GLY	A	908	-0.96	-16.991	31.91	1.00	26.6
703	CA	GLY	A	908	0.179	-16.436	31.193	1.00	25.34
704	C	GLY	A	908	0.834	-17.344	30.168	1.00	24.96
705	O	GLY	A	908	0.273	-18.371	29.785	1.00	24.83
706	N	ASN	A	909	2.025	-16.967	29.709	1.00	24.27
707	CA	ASN	A	909	2.716	-17.769	28.713	1.00	23.85
708	C	ASN	A	909	3.426	-18.965	29.347	1.00	23.59
709	O	ASN	A	909	3.795	-18.938	30.522	1.00	23.26
710	CB	ASN	A	909	3.69	-16.902	27.903	1.00	23.72
711	CG	ASN	A	909	4.922	-16.5	28.69	1.00	24.88
712	OD1	ASN	A	909	5.78	-17.333	29.001	1.00	24.46
713	ND2	ASN	A	909	5.02	-15.22	29.008	1.00	22.81
714	N	LEU	A	910	3.594	-20.017	28.55	1.00	23.4
715	CA	LEU	A	910	4.204	-21.261	29	1.00	21.84
716	C	LEU	A	910	5.619	-21.166	29.566	1.00	21.76
717	O	LEU	A	910	5.95	-21.894	30.501	1.00	20.41
718	CB	LEU	A	910	4.176	-22.282	27.86	1.00	19.8
719	CG	LEU	A	910	4.717	-23.688	28.128	1.00	19.35
720	CD1	LEU	A	910	3.942	-24.347	29.269	1.00	16.95
721	CD2	LEU	A	910	4.603	-24.514	26.846	1.00	18.26
722	N	LEU	A	911	6.452	-20.291	29.006	1.00	21.91
723	CA	LEU	A	911	7.82	-20.163	29.496	1.00	23.58
724	C	LEU	A	911	7.823	-19.709	30.952	1.00	24.17
725	O	LEU	A	911	8.464	-20.326	31.803	1.00	24.94
726	CB	LEU	A	911	8.631	-19.182	28.638	1.00	21.42
727	CG	LEU	A	911	10.119	-19.053	29.035	1.00	22.27
728	CD1	LEU	A	911	10.801	-20.423	29.014	1.00	19.43
729	CD2	LEU	A	911	10.833	-18.107	28.082	1.00	20.94
730	N	ASP	A	912	7.095	-18.639	31.24	1.00	25.51
731	CA	ASP	A	912	7.037	-18.136	32.6	1.00	27.7
732	C	ASP	A	912	6.34	-19.152	33.501	1.00	26.19
733	O	ASP	A	912	6.693	-19.298	34.67	1.00	27.16
734	CB	ASP	A	912	6.317	-16.775	32.651	1.00	31.26
735	CG	ASP	A	912	7	-15.714	31.779	1.00	36.96
736	OD1	ASP	A	912	8.244	-15.756	31.626	1.00	40.23
737	OD2	ASP	A	912	6.296	-14.821	31.252	1.00	39.36
738	N	PHE	A	913	5.363	-19.869	32.961	1.00	24.59
739	CA	PHE	A	913	4.657	-20.863	33.76	1.00	24.11
740	C	PHE	A	913	5.607	-21.999	34.173	1.00	24.35

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

741	O	PHE	A	913	5.561	-22.477	35.309	1.00	23.73
742	CB	PHE	A	913	3.473	-21.432	32.978	1.00	25.04
743	CG	PHE	A	913	2.486	-22.166	33.837	1.00	25.98
744	CD1	PHE	A	913	1.736	-21.482	34.789	1.00	26.55
745	CD2	PHE	A	913	2.314	-23.541	33.707	1.00	27.18
746	CE1	PHE	A	913	0.818	-22.162	35.609	1.00	28.73
747	CE2	PHE	A	913	1.403	-24.234	34.517	1.00	28.16
748	CZ	PHE	A	913	0.653	-23.542	35.47	1.00	28.89
749	N	LEU	A	914	6.457	-22.426	33.24	1.00	23.42
750	CA	LEU	A	914	7.427	-23.485	33.49	1.00	24.21
751	C	LEU	A	914	8.461	-23.032	34.527	1.00	25.19
752	O	LEU	A	914	8.82	-23.787	35.431	1.00	26.22
753	CB	LEU	A	914	8.159	-23.849	32.196	1.00	22.94
754	CG	LEU	A	914	7.409	-24.548	31.058	1.00	23.12
755	CD1	LEU	A	914	8.297	-24.558	29.82	1.00	22.24
756	CD2	LEU	A	914	7.029	-25.966	31.47	1.00	21.59
757	N	ARG	A	915	8.943	-21.801	34.382	1.00	25.1
758	CA	ARG	A	915	9.94	-21.257	35.302	1.00	26
759	C	ARG	A	915	9.366	-21.034	36.699	1.00	26.11
760	O	ARG	A	915	10.057	-21.221	37.693	1.00	25.71
761	CB	ARG	A	915	10.52	-19.959	34.728	1.00	23.15
762	CG	ARG	A	915	11.345	-20.232	33.482	1.00	24.97
763	CD	ARG	A	915	11.919	-18.987	32.83	1.00	24.93
764	NE	ARG	A	915	12.879	-19.371	31.795	1.00	25.91
765	CZ	ARG	A	915	13.473	-18.523	30.961	1.00	25.04
766	NH1	ARG	A	915	14.334	-18.975	30.057	1.00	24.14
767	NH2	ARG	A	915	13.202	-17.226	31.026	1.00	24.65
768	N	LYS	A	916	8.097	-20.651	36.772	1.00	27.35
769	CA	LYS	A	916	7.462	-20.437	38.065	1.00	29.22
770	C	LYS	A	916	7.172	-21.755	38.779	1.00	28.6
771	O	LYS	A	916	6.765	-21.753	39.936	1.00	29.81
772	CB	LYS	A	916	6.158	-19.65	37.903	1.00	30.24
773	CG	LYS	A	916	6.348	-18.181	37.565	1.00	34.72
774	CD	LYS	A	916	5.002	-17.465	37.499	1.00	37.62
775	CE	LYS	A	916	5.17	-15.999	37.131	1.00	38.34
776	NZ	LYS	A	916	5.962	-15.282	38.156	1.00	41.72
777	N	SER	A	917	7.375	-22.878	38.093	1.00	28.5
778	CA	SER	A	917	7.125	-24.183	38.707	1.00	27.99
779	C	SER	A	917	8.37	-24.756	39.39	1.00	27.82

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

780	O	SER	A	917	8.286	-25.782	40.058	1.00	27.8
781	CB	SER	A	917	6.621	-25.192	37.67	1.00	28.16
782	OG	SER	A	917	7.681	-25.681	36.864	1.00	27.17
783	N	ARG	A	918	9.517	-24.101	39.218	1.00	27.66
784	CA	ARG	A	918	10.758	-24.565	39.838	1.00	29
785	C	ARG	A	918	10.7	-24.284	41.341	1.00	30.2
786	O	ARG	A	918	11.413	-23.43	41.862	1.00	29.77
787	CB	ARG	A	918	11.959	-23.857	39.207	1.00	28.03
788	CG	ARG	A	918	12.199	-24.239	37.756	1.00	25.72
789	CD	ARG	A	918	13.451	-23.576	37.213	1.00	25.04
790	NE	ARG	A	918	13.744	-24.023	35.854	1.00	25.72
791	CZ	ARG	A	918	14.89	-23.801	35.22	1.00	24.79
792	NH1	ARG	A	918	15.061	-24.25	33.983	1.00	24.35
793	NH2	ARG	A	918	15.868	-23.141	35.825	1.00	22.99
794	N	VAL	A	919	9.835	-25.028	42.019	1.00	32.21
795	CA	VAL	A	919	9.59	-24.889	43.448	1.00	34.37
796	C	VAL	A	919	10.835	-24.992	44.329	1.00	35.24
797	O	VAL	A	919	10.89	-24.413	45.414	1.00	34.88
798	CB	VAL	A	919	8.543	-25.934	43.899	1.00	34.39
799	CG1	VAL	A	919	9.096	-27.337	43.716	1.00	34.31
800	CG2	VAL	A	919	8.144	-25.685	45.335	1.00	36.47
801	N	LEU	A	920	11.837	-25.723	43.862	1.00	37.18
802	CA	LEU	A	920	13.067	-25.886	44.622	1.00	38.69
803	C	LEU	A	920	13.763	-24.532	44.781	1.00	40.29
804	O	LEU	A	920	14.71	-24.395	45.559	1.00	41.25
805	CB	LEU	A	920	13.98	-26.883	43.909	1.00	38.61
806	CG	LEU	A	920	15.178	-27.479	44.646	1.00	38.61
807	CD1	LEU	A	920	14.748	-28.121	45.957	1.00	37.93
808	CD2	LEU	A	920	15.829	-28.51	43.74	1.00	37.75
809	N	GLU	A	921	13.285	-23.532	44.044	1.00	40.63
810	CA	GLU	A	921	13.856	-22.192	44.116	1.00	41.71
811	C	GLU	A	921	12.85	-21.187	44.655	1.00	41.25
812	O	GLU	A	921	13.218	-20.234	45.341	1.00	42.05
813	CB	GLU	A	921	14.336	-21.728	42.74	1.00	43.33
814	CG	GLU	A	921	15.486	-22.54	42.188	1.00	47.41
815	CD	GLU	A	921	16.133	-21.893	40.979	1.00	49.65
816	OE1	GLU	A	921	15.435	-21.687	39.962	1.00	50.98
817	OE2	GLU	A	921	17.346	-21.592	41.047	1.00	51.05
818	N	THR	A	922	11.578	-21.4	44.346	1.00	40.04

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

819	CA	THR	A	922	10.541	-20.488	44.798	1.00	39.04
820	C	THR	A	922	10.043	-20.831	46.197	1.00	38.98
821	O	THR	A	922	9.596	-19.948	46.924	1.00	40.08
822	CB	THR	A	922	9.35	-20.473	43.818	1.00	39
823	OG1	THR	A	922	8.634	-21.712	43.907	1.00	38.18
824	CG2	THR	A	922	9.853	-20.289	42.387	1.00	37.73
825	N	ASP	A	923	10.132	-22.105	46.578	1.00	38.09
826	CA	ASP	A	923	9.689	-22.553	47.902	1.00	37.32
827	C	ASP	A	923	10.315	-23.908	48.254	1.00	35.99
828	O	ASP	A	923	9.628	-24.928	48.31	1.00	35.07
829	CB	ASP	A	923	8.155	-22.643	47.929	1.00	39
830	CG	ASP	A	923	7.609	-23.122	49.273	1.00	41.21
831	OD1	ASP	A	923	8.368	-23.147	50.27	1.00	41.66
832	OD2	ASP	A	923	6.408	-23.466	49.332	1.00	42.49
833	N	PRO	A	924	11.636	-23.925	48.513	1.00	34.92
834	CA	PRO	A	924	12.382	-25.144	48.857	1.00	34.97
835	C	PRO	A	924	11.819	-26.012	49.987	1.00	34.48
836	O	PRO	A	924	12.03	-27.223	49.994	1.00	33.76
837	CB	PRO	A	924	13.796	-24.625	49.145	1.00	34.73
838	CG	PRO	A	924	13.572	-23.182	49.529	1.00	36.03
839	CD	PRO	A	924	12.512	-22.743	48.563	1.00	34.27
840	N	ALA	A	925	11.108	-25.411	50.935	1.00	35.1
841	CA	ALA	A	925	10.525	-26.192	52.022	1.00	35.97
842	C	ALA	A	925	9.485	-27.149	51.434	1.00	36.54
843	O	ALA	A	925	9.495	-28.35	51.713	1.00	36
844	CB	ALA	A	925	9.877	-25.266	53.048	1.00	36.01
845	N	PHE	A	926	8.593	-26.601	50.614	1.00	38.15
846	CA	PHE	A	926	7.552	-27.384	49.953	1.00	39.3
847	C	PHE	A	926	8.226	-28.44	49.089	1.00	39
848	O	PHE	A	926	7.826	-29.606	49.08	1.00	39.45
849	CB	PHE	A	926	6.7	-26.48	49.053	1.00	41.13
850	CG	PHE	A	926	5.699	-27.225	48.207	1.00	41.93
851	CD1	PHE	A	926	4.444	-27.553	48.711	1.00	42.38
852	CD2	PHE	A	926	6.019	-27.609	46.906	1.00	42.94
853	CE1	PHE	A	926	3.519	-28.252	47.932	1.00	42.44
854	CE2	PHE	A	926	5.105	-28.309	46.116	1.00	43.03
855	CZ	PHE	A	926	3.851	-28.632	46.633	1.00	43.17
856	N	ALA	A	927	9.253	-28.008	48.361	1.00	37.48
857	CA	ALA	A	927	10.009	-28.882	47.473	1.00	35.87

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

858	C	ALA	A	927	10.622	-30.06	48.221	1.00	35.27
859	O	ALA	A	927	10.467	-31.208	47.815	1.00	34.1
860	CB	ALA	A	927	11.101	-28.081	46.766	1.00	34.8
861	N	ILE	A	928	11.324	-29.773	49.313	1.00	36.13
862	CA	ILE	A	928	11.96	-30.827	50.099	1.00	36.42
863	C	ILE	A	928	10.914	-31.723	50.74	1.00	36.47
864	O	ILE	A	928	11.046	-32.946	50.73	1.00	37.25
865	CB	ILE	A	928	12.853	-30.242	51.218	1.00	36.93
866	CG1	ILE	A	928	14.023	-29.471	50.601	1.00	35.84
867	CG2	ILE	A	928	13.36	-31.365	52.123	1.00	37.06
868	CD1	ILE	A	928	14.881	-30.296	49.686	1.00	35.42
869	N	ALA	A	929	9.878	-31.11	51.299	1.00	36.88
870	CA	ALA	A	929	8.804	-31.853	51.949	1.00	36.86
871	C	ALA	A	929	8.073	-32.766	50.972	1.00	36.9
872	O	ALA	A	929	7.562	-33.815	51.355	1.00	38.1
873	CB	ALA	A	929	7.813	-30.881	52.589	1.00	37.02
874	N	ASN	A	930	8.027	-32.368	49.707	1.00	35.97
875	CA	ASN	A	930	7.337	-33.158	48.698	1.00	35.39
876	C	ASN	A	930	8.291	-33.865	47.748	1.00	34.56
877	O	ASN	A	930	7.864	-34.413	46.733	1.00	33.96
878	CB	ASN	A	930	6.373	-32.265	47.91	1.00	36.05
879	CG	ASN	A	930	5.187	-31.81	48.745	1.00	37.02
880	OD1	ASN	A	930	4.288	-32.596	49.041	1.00	37.77
881	ND2	ASN	A	930	5.19	-30.543	49.144	1.00	37.18
882	N	SER	A	931	9.578	-33.854	48.086	1.00	33.11
883	CA	SER	A	931	10.597	-34.498	47.264	1.00	32.84
884	C	SER	A	931	10.409	-34.186	45.777	1.00	31.49
885	O	SER	A	931	10.569	-35.066	44.926	1.00	30.49
886	CB	SER	A	931	10.552	-36.014	47.469	1.00	33.5
887	OG	SER	A	931	10.725	-36.343	48.834	1.00	37.31
888	N	THR	A	932	10.086	-32.935	45.463	1.00	29.58
889	CA	THR	A	932	9.868	-32.559	44.073	1.00	29.27
890	C	THR	A	932	10.518	-31.311	43.597	1.00	27.6
891	O	THR	A	932	10.924	-30.414	44.378	1.00	27.45
892	CB	THR	A	932	8.37	-32.358	43.8	1.00	29.49
893	OG1	THR	A	932	8.166	-32.19	42.395	1.00	32.12
894	CG2	THR	A	932	7.85	-31.134	44.525	1.00	28.32
895	N	ALA	A	933	10.91	-31.269	42.301	1.00	26.02
896	CA	ALA	A	933	11.616	-30.141	41.686	1.00	25.55

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

897	C	ALA	A	933	10.648	-29.26	40.91	1.00	25.42
898	O	ALA	A	933	11.05	-28.254	40.313	1.00	24.78
899	CB	ALA	A	933	12.72	-30.646	40.771	1.00	24.31
900	N	SER	A	934	9.372	-29.64	40.905	1.00	24.56
901	CA	SER	A	934	8.376	-28.871	40.178	1.00	26.03
902	C	SER	A	934	6.954	-29.121	40.658	1.00	26.27
903	O	SER	A	934	6.628	-30.207	41.131	1.00	26.27
904	CB	SER	A	934	8.461	-29.189	38.681	1.00	26.09
905	OG	SER	A	934	7.531	-28.411	37.946	1.00	28
906	N	THR	A	935	6.111	-28.103	40.536	1.00	26.46
907	CA	THR	A	935	4.714	-28.231	40.918	1.00	27.15
908	C	THR	A	935	4	-28.925	39.767	1.00	26.42
909	O	THR	A	935	2.822	-29.256	39.854	1.00	27.12
910	CB	THR	A	935	4.072	-26.857	41.157	1.00	28.19
911	OG1	THR	A	935	4.377	-25.991	40.054	1.00	28.39
912	CG2	THR	A	935	4.598	-26.247	42.457	1.00	27.95
913	N	LEU	A	936	4.738	-29.149	38.687	1.00	26.32
914	CA	LEU	A	936	4.194	-29.81	37.509	1.00	25.47
915	C	LEU	A	936	4.706	-31.245	37.441	1.00	25.2
916	O	LEU	A	936	5.89	-31.505	37.673	1.00	24.32
917	CB	LEU	A	936	4.605	-29.04	36.246	1.00	23.7
918	CG	LEU	A	936	4.088	-27.598	36.148	1.00	23.21
919	CD1	LEU	A	936	4.686	-26.893	34.926	1.00	19.89
920	CD2	LEU	A	936	2.569	-27.617	36.074	1.00	23.05
921	N	SER	A	937	3.812	-32.177	37.124	1.00	25.72
922	CA	SER	A	937	4.188	-33.582	37.024	1.00	25.4
923	C	SER	A	937	4.624	-33.915	35.603	1.00	25.64
924	O	SER	A	937	4.417	-33.129	34.68	1.00	26.32
925	CB	SER	A	937	3.006	-34.472	37.395	1.00	26.2
926	OG	SER	A	937	2.043	-34.47	36.355	1.00	25.43
927	N	SER	A	938	5.226	-35.087	35.437	1.00	25.65
928	CA	SER	A	938	5.674	-35.552	34.134	1.00	25.79
929	C	SER	A	938	4.482	-35.625	33.173	1.00	26.33
930	O	SER	A	938	4.598	-35.268	32.003	1.00	26
931	CB	SER	A	938	6.318	-36.933	34.269	1.00	25.7
932	OG	SER	A	938	6.699	-37.45	33.006	1.00	25.71
933	N	GLN	A	939	3.343	-36.099	33.673	1.00	26.84
934	CA	GLN	A	939	2.127	-36.209	32.864	1.00	27.76
935	C	GLN	A	939	1.664	-34.836	32.375	1.00	26.81

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

936	O	GLN	A	939	1.265	-34.679	31.22	1.00	27.38
937	CB	GLN	A	939	1	-36.863	33.68	1.00	28.83
938	CG	GLN	A	939	1.118	-38.373	33.808	1.00	34.01
939	CD	GLN	A	939	0.687	-39.101	32.544	1.00	34.97
940	OE1	GLN	A	939	1.324	-40.066	32.122	1.00	37.75
941	NE2	GLN	A	939	-0.406	-38.645	31.942	1.00	34.75
942	N	GLN	A	940	1.708	-33.846	33.262	1.00	25.14
943	CA	GLN	A	940	1.281	-32.5	32.909	1.00	24.64
944	C	GLN	A	940	2.202	-31.864	31.874	1.00	24.09
945	O	GLN	A	940	1.749	-31.146	30.982	1.00	24.26
946	CB	GLN	A	940	1.22	-31.63	34.163	1.00	24.75
947	CG	GLN	A	940	0.105	-32.009	35.12	1.00	26.7
948	CD	GLN	A	940	0.165	-31.22	36.413	1.00	29.61
949	OE1	GLN	A	940	1.166	-31.257	37.131	1.00	29.13
950	NE2	GLN	A	940	-0.909	-30.498	36.717	1.00	30.35
951	N	LEU	A	941	3.497	-32.126	31.997	1.00	23.07
952	CA	LEU	A	941	4.467	-31.575	31.066	1.00	23.05
953	C	LEU	A	941	4.255	-32.18	29.677	1.00	23.27
954	O	LEU	A	941	4.298	-31.477	28.674	1.00	22.26
955	CB	LEU	A	941	5.891	-31.855	31.563	1.00	22.49
956	CG	LEU	A	941	6.301	-31.141	32.861	1.00	22.55
957	CD1	LEU	A	941	7.66	-31.655	33.32	1.00	20.05
958	CD2	LEU	A	941	6.34	-29.63	32.643	1.00	20.32
959	N	LEU	A	942	4.02	-33.487	29.618	1.00	23.31
960	CA	LEU	A	942	3.797	-34.127	28.331	1.00	23.57
961	C	LEU	A	942	2.467	-33.676	27.726	1.00	22.67
962	O	LEU	A	942	2.347	-33.567	26.51	1.00	21.31
963	CB	LEU	A	942	3.852	-35.653	28.468	1.00	24.98
964	CG	LEU	A	942	5.253	-36.238	28.717	1.00	26.35
965	CD1	LEU	A	942	5.163	-37.758	28.719	1.00	27.72
966	CD2	LEU	A	942	6.231	-35.783	27.641	1.00	26.9
967	N	HIS	A	943	1.472	-33.409	28.571	1.00	22.5
968	CA	HIS	A	943	0.185	-32.927	28.075	1.00	24
969	C	HIS	A	943	0.34	-31.542	27.44	1.00	23.07
970	O	HIS	A	943	-0.402	-31.19	26.526	1.00	21.92
971	CB	HIS	A	943	-0.856	-32.871	29.2	1.00	27.24
972	CG	HIS	A	943	-1.588	-34.162	29.399	1.00	31.72
973	ND1	HIS	A	943	-2.296	-34.776	28.385	1.00	33.42
974	CD2	HIS	A	943	-1.689	-34.978	30.475	1.00	32.93



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975	CE1	HIS	A	943	-2.797	-35.914	28.828	1.00	33.62
976	NE2	HIS	A	943	-2.443	-36.061	30.092	1.00	33.99
977	N	PHE	A	944	1.299	-30.759	27.933	1.00	22.19
978	CA	PHE	A	944	1.557	-29.434	27.369	1.00	21.47
979	C	PHE	A	944	2.131	-29.652	25.973	1.00	20.47
980	O	PHE	A	944	1.734	-28.99	25.011	1.00	19.75
981	CB	PHE	A	944	2.572	-28.658	28.23	1.00	21.46
982	CG	PHE	A	944	1.971	-27.983	29.442	1.00	22.29
983	CD1	PHE	A	944	2.735	-27.781	30.588	1.00	21.9
984	CD2	PHE	A	944	0.654	-27.52	29.427	1.00	22.87
985	CE1	PHE	A	944	2.203	-27.129	31.7	1.00	22.92
986	CE2	PHE	A	944	0.11	-26.866	30.533	1.00	23.38
987	CZ	PHE	A	944	0.886	-26.669	31.672	1.00	23.34
988	N	ALA	A	945	3.07	-30.593	25.872	1.00	18.9
989	CA	ALA	A	945	3.7	-30.907	24.59	1.00	19.27
990	C	ALA	A	945	2.668	-31.451	23.601	1.00	18.77
991	O	ALA	A	945	2.68	-31.093	22.425	1.00	18.19
992	CB	ALA	A	945	4.833	-31.925	24.79	1.00	17.98
993	N	ALA	A	946	1.773	-32.308	24.089	1.00	17.94
994	CA	ALA	A	946	0.731	-32.895	23.254	1.00	18.09
995	C	ALA	A	946	-0.22	-31.812	22.768	1.00	17.61
996	O	ALA	A	946	-0.63	-31.823	21.608	1.00	18.41
997	CB	ALA	A	946	-0.041	-33.971	24.033	1.00	16.95
998	N	ASP	A	947	-0.569	-30.883	23.655	1.00	19.2
999	CA	ASP	A	947	-1.46	-29.77	23.304	1.00	19.63
1000	C	ASP	A	947	-0.901	-28.958	22.127	1.00	19.3
1001	O	ASP	A	947	-1.613	-28.657	21.174	1.00	19.9
1002	CB	ASP	A	947	-1.641	-28.822	24.495	1.00	20.36
1003	CG	ASP	A	947	-2.64	-29.337	25.515	1.00	24.18
1004	OD1	ASP	A	947	-2.677	-28.783	26.639	1.00	25.81
1005	OD2	ASP	A	947	-3.394	-30.279	25.202	1.00	25.86
1006	N	VAL	A	948	0.372	-28.596	22.202	1.00	17.69
1007	CA	VAL	A	948	0.98	-27.81	21.142	1.00	18.56
1008	C	VAL	A	948	1.056	-28.608	19.845	1.00	19.37
1009	O	VAL	A	948	0.793	-28.074	18.773	1.00	19.72
1010	CB	VAL	A	948	2.397	-27.332	21.548	1.00	17.83
1011	CG1	VAL	A	948	3.013	-26.49	20.43	1.00	14.69
1012	CG2	VAL	A	948	2.309	-26.518	22.828	1.00	16.69
1013	N	ALA	A	949	1.411	-29.886	19.947	1.00	19.69

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

1014	CA	ALA	A	949	1.51	-30.739	18.772	1.00	20.88
1015	C	ALA	A	949	0.134	-30.899	18.105	1.00	20.67
1016	O	ALA	A	949	0.027	-30.9	16.884	1.00	19.04
1017	CB	ALA	A	949	2.073	-32.11	19.164	1.00	20.28
1018	N	ARG	A	950	-0.909	-31.035	18.918	1.00	21.37
1019	CA	ARG	A	950	-2.264	-31.192	18.405	1.00	22.99
1020	C	ARG	A	950	-2.665	-29.896	17.71	1.00	23.96
1021	O	ARG	A	950	-3.267	-29.913	16.635	1.00	24.86
1022	CB	ARG	A	950	-3.235	-31.5	19.554	1.00	23.59
1023	CG	ARG	A	950	-4.619	-31.958	19.1	1.00	23.76
1024	CD	ARG	A	950	-5.557	-32.196	20.291	1.00	22.56
1025	NE	ARG	A	950	-5.004	-33.164	21.233	1.00	23.34
1026	CZ	ARG	A	950	-4.415	-32.846	22.383	1.00	24.54
1027	NH1	ARG	A	950	-3.934	-33.8	23.166	1.00	23.35
1028	NH2	ARG	A	950	-4.325	-31.577	22.765	1.00	24.9
1029	N	GLY	A	951	-2.309	-28.772	18.326	1.00	23.55
1030	CA	GLY	A	951	-2.63	-27.48	17.752	1.00	22.75
1031	C	GLY	A	951	-1.867	-27.192	16.469	1.00	23.11
1032	O	GLY	A	951	-2.415	-26.577	15.551	1.00	22.36
1033	N	MET	A	952	-0.609	-27.626	16.39	1.00	21.96
1034	CA	MET	A	952	0.186	-27.387	15.186	1.00	22.55
1035	C	MET	A	952	-0.227	-28.308	14.047	1.00	22.85
1036	O	MET	A	952	-0.034	-27.985	12.874	1.00	22.17
1037	CB	MET	A	952	1.683	-27.552	15.468	1.00	22.99
1038	CG	MET	A	952	2.328	-26.334	16.122	1.00	22.86
1039	SD	MET	A	952	1.955	-24.788	15.245	1.00	24.9
1040	CE	MET	A	952	2.817	-25.03	13.71	1.00	21.59
1041	N	ASP	A	953	-0.776	-29.466	14.394	1.00	23.16
1042	CA	ASP	A	953	-1.244	-30.399	13.382	1.00	24.56
1043	C	ASP	A	953	-2.433	-29.704	12.724	1.00	24.84
1044	O	ASP	A	953	-2.547	-29.653	11.502	1.00	26.22
1045	CB	ASP	A	953	-1.683	-31.709	14.037	1.00	26.86
1046	CG	ASP	A	953	-2.371	-32.649	13.066	1.00	26.98
1047	OD1	ASP	A	953	-3.51	-33.057	13.36	1.00	29.54
1048	OD2	ASP	A	953	-1.779	-32.985	12.023	1.00	26.23
1049	N	TYR	A	954	-3.306	-29.136	13.546	1.00	24.2
1050	CA	TYR	A	954	-4.467	-28.424	13.036	1.00	24.64
1051	C	TYR	A	954	-4.061	-27.258	12.113	1.00	25.13
1052	O	TYR	A	954	-4.563	-27.139	10.998	1.00	26.05

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

1053	CB	TYR	A	954	-5.305	-27.901	14.207	1.00	25.17
1054	CG	TYR	A	954	-6.419	-26.964	13.793	1.00	27.11
1055	CD1	TYR	A	954	-7.602	-27.448	13.216	1.00	26.91
1056	CD2	TYR	A	954	-6.273	-25.59	13.941	1.00	26.83
1057	CE1	TYR	A	954	-8.612	-26.57	12.795	1.00	27.1
1058	CE2	TYR	A	954	-7.267	-24.709	13.528	1.00	27.98
1059	CZ	TYR	A	954	-8.432	-25.201	12.955	1.00	27.85
1060	OH	TYR	A	954	-9.396	-24.306	12.552	1.00	28.21
1061	N	LEU	A	955	-3.152	-26.403	12.576	1.00	23.91
1062	CA	LEU	A	955	-2.697	-25.252	11.79	1.00	23.82
1063	C	LEU	A	955	-1.922	-25.639	10.529	1.00	24.4
1064	O	LEU	A	955	-2.144	-25.083	9.447	1.00	23.79
1065	CB	LEU	A	955	-1.824	-24.335	12.66	1.00	22.43
1066	CG	LEU	A	955	-2.549	-23.635	13.817	1.00	23.08
1067	CD1	LEU	A	955	-1.543	-22.953	14.738	1.00	24.18
1068	CD2	LEU	A	955	-3.535	-22.621	13.256	1.00	24.39
1069	N	SER	A	956	-0.998	-26.577	10.688	1.00	24.96
1070	CA	SER	A	956	-0.175	-27.063	9.59	1.00	27.37
1071	C	SER	A	956	-1.065	-27.632	8.478	1.00	28.44
1072	O	SER	A	956	-0.856	-27.364	7.292	1.00	27.37
1073	CB	SER	A	956	0.77	-28.15	10.115	1.00	27.52
1074	OG	SER	A	956	1.505	-28.74	9.065	1.00	31.76
1075	N	GLN	A	957	-2.059	-28.414	8.878	1.00	29.42
1076	CA	GLN	A	957	-2.985	-29.026	7.937	1.00	32.18
1077	C	GLN	A	957	-3.702	-27.949	7.125	1.00	31.66
1078	O	GLN	A	957	-4.159	-28.201	6.011	1.00	29.88
1079	CB	GLN	A	957	-4.008	-29.879	8.691	1.00	36.81
1080	CG	GLN	A	957	-4.906	-30.715	7.798	1.00	44.3
1081	CD	GLN	A	957	-4.126	-31.745	7	1.00	48.83
1082	OE1	GLN	A	957	-3.347	-32.521	7.563	1.00	51.15
1083	NE2	GLN	A	957	-4.337	-31.765	5.681	1.00	50.11
1084	N	LYS	A	958	-3.792	-26.743	7.677	1.00	30.67
1085	CA	LYS	A	958	-4.449	-25.662	6.964	1.00	30.08
1086	C	LYS	A	958	-3.463	-24.694	6.327	1.00	29.03
1087	O	LYS	A	958	-3.779	-23.532	6.099	1.00	29.33
1088	CB	LYS	A	958	-5.422	-24.931	7.889	1.00	31.03
1089	CG	LYS	A	958	-6.452	-25.881	8.491	1.00	33.3
1090	CD	LYS	A	958	-7.838	-25.282	8.568	1.00	36.85
1091	CE	LYS	A	958	-7.922	-24.152	9.561	1.00	38.23

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1092	NZ	LYS	A	958	-9.295	-23.568	9.532	1.00	41.8
1093	N	GLN	A	959	-2.261	-25.187	6.049	1.00	28.89
1094	CA	GLN	A	959	-1.228	-24.4	5.389	1.00	29.36
1095	C	GLN	A	959	-0.556	-23.296	6.213	1.00	27.95
1096	O	GLN	A	959	0.222	-22.506	5.673	1.00	28
1097	CB	GLN	A	959	-1.807	-23.795	4.104	1.00	34.14
1098	CG	GLN	A	959	-2.446	-24.806	3.152	1.00	38.82
1099	CD	GLN	A	959	-1.425	-25.728	2.494	1.00	43.6
1100	OE1	GLN	A	959	-0.561	-25.281	1.725	1.00	45.2
1101	NE2	GLN	A	959	-1.519	-27.023	2.792	1.00	44.69
1102	N	PHE	A	960	-0.844	-23.22	7.505	1.00	25.63
1103	CA	PHE	A	960	-0.207	-22.188	8.32	1.00	25.08
1104	C	PHE	A	960	1.249	-22.536	8.62	1.00	23.3
1105	O	PHE	A	960	1.592	-23.706	8.787	1.00	23.12
1106	CB	PHE	A	960	-0.94	-21.99	9.656	1.00	25.96
1107	CG	PHE	A	960	-2.236	-21.237	9.541	1.00	26.42
1108	CD1	PHE	A	960	-3.435	-21.91	9.317	1.00	26.63
1109	CD2	PHE	A	960	-2.258	-19.849	9.656	1.00	26.53
1110	CE1	PHE	A	960	-4.645	-21.21	9.209	1.00	25.75
1111	CE2	PHE	A	960	-3.458	-19.143	9.549	1.00	26.35
1112	CZ	PHE	A	960	-4.656	-19.827	9.324	1.00	25.48
1113	N	ILE	A	961	2.092	-21.509	8.665	1.00	22.09
1114	CA	ILE	A	961	3.51	-21.642	8.989	1.00	21.62
1115	C	ILE	A	961	3.711	-20.628	10.118	1.00	21.62
1116	O	ILE	A	961	3.569	-19.426	9.906	1.00	20.73
1117	CB	ILE	A	961	4.42	-21.27	7.79	1.00	21.99
1118	CG1	ILE	A	961	4.14	-22.208	6.61	1.00	21.69
1119	CG2	ILE	A	961	5.888	-21.392	8.191	1.00	18.31
1120	CD1	ILE	A	961	4.906	-21.849	5.327	1.00	22.34
1121	N	HIS	A	962	4.027	-21.12	11.311	1.00	21.26
1122	CA	HIS	A	962	4.195	-20.27	12.488	1.00	22.26
1123	C	HIS	A	962	5.427	-19.366	12.46	1.00	23.24
1124	O	HIS	A	962	5.315	-18.166	12.704	1.00	22.37
1125	CB	HIS	A	962	4.203	-21.141	13.748	1.00	22.04
1126	CG	HIS	A	962	3.98	-20.374	15.012	1.00	21.56
1127	ND1	HIS	A	962	4.956	-19.59	15.591	1.00	20.49
1128	CD2	HIS	A	962	2.876	-20.237	15.787	1.00	21.34
1129	CE1	HIS	A	962	4.461	-19.001	16.666	1.00	22.34
1130	NE2	HIS	A	962	3.201	-19.376	16.807	1.00	23.05

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

1131	N	ARG	A	963	6.592	-19.947	12.173	1.00	24.02
1132	CA	ARG	A	963	7.859	-19.211	12.085	1.00	25.85
1133	C	ARG	A	963	8.57	-18.911	13.411	1.00	25.62
1134	O	ARG	A	963	9.794	-18.76	13.437	1.00	25.81
1135	CB	ARG	A	963	7.678	-17.871	11.345	1.00	27.66
1136	CG	ARG	A	963	7.077	-17.936	9.937	1.00	29.93
1137	CD	ARG	A	963	7.308	-16.607	9.19	1.00	31.38
1138	NE	ARG	A	963	7.021	-15.439	10.024	1.00	34.29
1139	CZ	ARG	A	963	5.801	-14.991	10.325	1.00	36.41
1140	NH1	ARG	A	963	4.718	-15.599	9.856	1.00	36.37
1141	NH2	ARG	A	963	5.66	-13.943	11.127	1.00	38.14
1142	N	ASP	A	964	7.815	-18.807	14.501	1.00	25.89
1143	CA	ASP	A	964	8.401	-18.485	15.798	1.00	25.4
1144	C	ASP	A	964	7.811	-19.347	16.913	1.00	24.87
1145	O	ASP	A	964	7.343	-18.841	17.933	1.00	23.96
1146	CB	ASP	A	964	8.184	-16.993	16.092	1.00	28.01
1147	CG	ASP	A	964	8.973	-16.502	17.302	1.00	31.45
1148	OD1	ASP	A	964	9.94	-17.185	17.709	1.00	31.29
1149	OD2	ASP	A	964	8.63	-15.424	17.837	1.00	33.52
1150	N	LEU	A	965	7.854	-20.659	16.713	1.00	23.88
1151	CA	LEU	A	965	7.314	-21.603	17.681	1.00	24.62
1152	C	LEU	A	965	8.283	-21.729	18.86	1.00	24.63
1153	O	LEU	A	965	9.433	-22.125	18.689	1.00	26.99
1154	CB	LEU	A	965	7.108	-22.955	16.998	1.00	25.23
1155	CG	LEU	A	965	6.06	-23.924	17.538	1.00	26.24
1156	CD1	LEU	A	965	4.752	-23.193	17.829	1.00	25
1157	CD2	LEU	A	965	5.838	-25.023	16.498	1.00	25.01
1158	N	ALA	A	966	7.808	-21.391	20.052	1.00	22.67
1159	CA	ALA	A	966	8.632	-21.433	21.256	1.00	20.88
1160	C	ALA	A	966	7.707	-21.265	22.449	1.00	20.11
1161	O	ALA	A	966	6.588	-20.769	22.295	1.00	18.73
1162	CB	ALA	A	966	9.658	-20.297	21.226	1.00	21.39
1163	N	ALA	A	967	8.177	-21.653	23.633	1.00	18.75
1164	CA	ALA	A	967	7.365	-21.571	24.848	1.00	19.33
1165	C	ALA	A	967	6.768	-20.19	25.128	1.00	20.1
1166	O	ALA	A	967	5.648	-20.083	25.642	1.00	19.27
1167	CB	ALA	A	967	8.184	-22.041	26.051	1.00	19.85
1168	N	ARG	A	968	7.515	-19.138	24.8	1.00	20.79
1169	CA	ARG	A	968	7.044	-17.777	25.023	1.00	20.8

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

1170	C	ARG	A	968	5.818	-17.478	24.168	1.00	20.23
1171	O	ARG	A	968	5.064	-16.55	24.464	1.00	20.38
1172	CB	ARG	A	968	8.146	-16.762	24.689	1.00	22.09
1173	CG	ARG	A	968	8.613	-16.833	23.245	1.00	22.25
1174	CD	ARG	A	968	9.6	-15.727	22.9	1.00	24.41
1175	NE	ARG	A	968	10.201	-15.957	21.588	1.00	25.14
1176	CZ	ARG	A	968	11.152	-16.855	21.353	1.00	27.01
1177	NH1	ARG	A	968	11.621	-17.6	22.342	1.00	29.68
1178	NH2	ARG	A	968	11.625	-17.026	20.129	1.00	28.05
1179	N	ASN	A	969	5.631	-18.253	23.101	1.00	19.17
1180	CA	ASN	A	969	4.495	-18.046	22.207	1.00	19.5
1181	C	ASN	A	969	3.371	-19.057	22.41	1.00	19.78
1182	O	ASN	A	969	2.517	-19.245	21.539	1.00	20.1
1183	CB	ASN	A	969	4.949	-18.057	20.742	1.00	19.74
1184	CG	ASN	A	969	5.424	-16.695	20.269	1.00	20.1
1185	OD1	ASN	A	969	4.892	-15.669	20.687	1.00	19.59
1186	ND2	ASN	A	969	6.404	-16.679	19.372	1.00	19.71
1187	N	ILE	A	970	3.385	-19.713	23.563	1.00	19.2
1188	CA	ILE	A	970	2.354	-20.674	23.916	1.00	19.03
1189	C	ILE	A	970	1.725	-20.123	25.189	1.00	20.71
1190	O	ILE	A	970	2.436	-19.718	26.116	1.00	21.54
1191	CB	ILE	A	970	2.94	-22.071	24.23	1.00	19.22
1192	CG1	ILE	A	970	3.686	-22.629	23.008	1.00	19.08
1193	CG2	ILE	A	970	1.822	-23.016	24.683	1.00	18.95
1194	CD1	ILE	A	970	2.838	-22.754	21.724	1.00	17.97
1195	N	LEU	A	971	0.401	-20.085	25.238	1.00	19.7
1196	CA	LEU	A	971	-0.274	-19.595	26.426	1.00	20.19
1197	C	LEU	A	971	-0.974	-20.727	27.186	1.00	20.79
1198	O	LEU	A	971	-1.441	-21.706	26.592	1.00	19.95
1199	CB	LEU	A	971	-1.254	-18.482	26.03	1.00	20.93
1200	CG	LEU	A	971	-0.42	-17.309	25.47	1.00	23.31
1201	CD1	LEU	A	971	-0.93	-16.885	24.105	1.00	20.37
1202	CD2	LEU	A	971	-0.392	-16.158	26.466	1.00	20.87
1203	N	VAL	A	972	-1.001	-20.609	28.51	1.00	21.3
1204	CA	VAL	A	972	-1.649	-21.599	29.359	1.00	22.27
1205	C	VAL	A	972	-3.021	-21.028	29.702	1.00	23.79
1206	O	VAL	A	972	-3.147	-20.153	30.56	1.00	23.04
1207	CB	VAL	A	972	-0.811	-21.848	30.637	1.00	23.12
1208	CG1	VAL	A	972	-1.455	-22.937	31.496	1.00	21.2

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

1209	CG2	VAL	A	972	0.608	-22.26	30.242	1.00	21.66
1210	N	GLY	A	973	-4.05	-21.522	29.018	1.00	25.18
1211	CA	GLY	A	973	-5.39	-21.002	29.236	1.00	29.28
1212	C	GLY	A	973	-6.263	-21.711	30.254	1.00	31.37
1213	O	GLY	A	973	-5.766	-22.373	31.161	1.00	30.01
1214	N	GLU	A	974	-7.576	-21.545	30.101	1.00	34.07
1215	CA	GLU	A	974	-8.553	-22.165	30.993	1.00	37.03
1216	C	GLU	A	974	-8.291	-23.646	31.165	1.00	35.78
1217	O	GLU	A	974	-7.992	-24.347	30.198	1.00	36.41
1218	CB	GLU	A	974	-9.97	-21.993	30.451	1.00	40.53
1219	CG	GLU	A	974	-10.641	-20.694	30.822	1.00	46.5
1220	CD	GLU	A	974	-12.127	-20.732	30.519	1.00	50.09
1221	OE1	GLU	A	974	-12.489	-20.918	29.336	1.00	52.44
1222	OE2	GLU	A	974	-12.933	-20.59	31.465	1.00	52.73
1223	N	ASN	A	975	-8.429	-24.116	32.4	1.00	34.98
1224	CA	ASN	A	975	-8.204	-25.517	32.736	1.00	33.91
1225	C	ASN	A	975	-6.807	-25.974	32.334	1.00	31.64
1226	O	ASN	A	975	-6.564	-27.156	32.113	1.00	30.9
1227	CB	ASN	A	975	-9.264	-26.404	32.073	1.00	36.61
1228	CG	ASN	A	975	-10.676	-26.078	32.545	1.00	40.18
1229	OD1	ASN	A	975	-11.329	-25.174	32.018	1.00	41.74
1230	ND2	ASN	A	975	-11.148	-26.81	33.556	1.00	41.5
1231	N	TYR	A	976	-5.894	-25.017	32.25	1.00	29.84
1232	CA	TYR	A	976	-4.503	-25.273	31.901	1.00	28.7
1233	C	TYR	A	976	-4.268	-25.892	30.532	1.00	27.18
1234	O	TYR	A	976	-3.32	-26.642	30.343	1.00	28.12
1235	CB	TYR	A	976	-3.839	-26.122	32.986	1.00	29.59
1236	CG	TYR	A	976	-3.929	-25.481	34.353	1.00	31.41
1237	CD1	TYR	A	976	-5.062	-25.654	35.153	1.00	31.5
1238	CD2	TYR	A	976	-2.914	-24.645	34.819	1.00	29.79
1239	CE1	TYR	A	976	-5.183	-25.005	36.384	1.00	31.98
1240	CE2	TYR	A	976	-3.022	-23.995	36.041	1.00	30.87
1241	CZ	TYR	A	976	-4.158	-24.175	36.819	1.00	32.68
1242	OH	TYR	A	976	-4.282	-23.5	38.015	1.00	33.12
1243	N	VAL	A	977	-5.138	-25.571	29.582	1.00	25.67
1244	CA	VAL	A	977	-5.004	-26.059	28.217	1.00	25.39
1245	C	VAL	A	977	-4.046	-25.121	27.46	1.00	24.71
1246	O	VAL	A	977	-4.312	-23.928	27.345	1.00	24.11
1247	CB	VAL	A	977	-6.374	-26.057	27.494	1.00	25.95

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

1248	CG1	VAL	A	977	-6.194	-26.392	26.019	1.00	24.68
1249	CG2	VAL	A	977	-7.315	-27.06	28.162	1.00	25.19
1250	N	ALA	A	978	-2.941	-25.661	26.95	1.00	23.33
1251	CA	ALA	A	978	-1.97	-24.862	26.203	1.00	21.4
1252	C	ALA	A	978	-2.536	-24.416	24.855	1.00	21.9
1253	O	ALA	A	978	-3.055	-25.233	24.087	1.00	21.21
1254	CB	ALA	A	978	-0.693	-25.658	25.984	1.00	19.43
1255	N	LYS	A	979	-2.426	-23.118	24.572	1.00	21.38
1256	CA	LYS	A	979	-2.922	-22.557	23.319	1.00	21.5
1257	C	LYS	A	979	-1.819	-21.831	22.564	1.00	22.03
1258	O	LYS	A	979	-1.095	-21.018	23.134	1.00	23.81
1259	CB	LYS	A	979	-4.076	-21.598	23.6	1.00	20.58
1260	CG	LYS	A	979	-5.332	-22.291	24.122	1.00	20.31
1261	CD	LYS	A	979	-6.287	-21.298	24.774	1.00	19.82
1262	CE	LYS	A	979	-7.552	-21.996	25.234	1.00	22.11
1263	NZ	LYS	A	979	-8.372	-22.39	24.056	1.00	23.18
1264	N	ILE	A	980	-1.694	-22.127	21.278	1.00	21.64
1265	CA	ILE	A	980	-0.673	-21.493	20.448	1.00	21.67
1266	C	ILE	A	980	-1.027	-20.044	20.075	1.00	22.7
1267	O	ILE	A	980	-2.141	-19.777	19.613	1.00	22.34
1268	CB	ILE	A	980	-0.474	-22.294	19.15	1.00	20.85
1269	CG1	ILE	A	980	-0.062	-23.724	19.497	1.00	19.41
1270	CG2	ILE	A	980	0.563	-21.612	18.252	1.00	16.97
1271	CD1	ILE	A	980	-0.101	-24.662	18.336	1.00	21.04
1272	N	ALA	A	981	-0.09	-19.115	20.293	1.00	22.22
1273	CA	ALA	A	981	-0.313	-17.716	19.919	1.00	23.04
1274	C	ALA	A	981	-0.272	-17.727	18.389	1.00	23.75
1275	O	ALA	A	981	0.69	-18.216	17.788	1.00	22.49
1276	CB	ALA	A	981	0.79	-16.814	20.482	1.00	21.55
1277	N	ASP	A	982	-1.306	-17.171	17.766	1.00	24.84
1278	CA	ASP	A	982	-1.425	-17.201	16.314	1.00	24.92
1279	C	ASP	A	982	-1.654	-15.88	15.575	1.00	25.48
1280	O	ASP	A	982	-2.41	-15.839	14.6	1.00	26.48
1281	CB	ASP	A	982	-2.542	-18.182	15.96	1.00	23.62
1282	CG	ASP	A	982	-3.795	-17.951	16.782	1.00	23.1
1283	OD1	ASP	A	982	-4.693	-18.82	16.766	1.00	23.37
1284	OD2	ASP	A	982	-3.887	-16.895	17.443	1.00	21.87
1285	N	PHE	A	983	-1.002	-14.815	16.023	1.00	24.4
1286	CA	PHE	A	983	-1.134	-13.519	15.365	1.00	25.08



TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

1287	C	PHE	A	983	0.032	-13.337	14.396	1.00	25.12
1288	O	PHE	A	983	1.169	-13.665	14.723	1.00	24.45
1289	CB	PHE	A	983	-1.106	-12.377	16.383	1.00	24.8
1290	CG	PHE	A	983	-1.348	-11.021	15.771	1.00	25.18
1291	CD1	PHE	A	983	-2.644	-10.589	15.497	1.00	25.04
1292	CD2	PHE	A	983	-0.28	-10.203	15.41	1.00	25.27
1293	CE1	PHE	A	983	-2.872	-9.368	14.872	1.00	24.91
1294	CE2	PHE	A	983	-0.498	-8.974	14.78	1.00	25.31
1295	CZ	PHE	A	983	-1.795	-8.559	14.512	1.00	25.38
1296	N	GLY	A	984	-0.253	-12.827	13.203	1.00	25.59
1297	CA	GLY	A	984	0.802	-12.599	12.228	1.00	25.41
1298	C	GLY	A	984	1.464	-13.83	11.635	1.00	26.25
1299	O	GLY	A	984	2.622	-13.773	11.22	1.00	27.64
1300	N	LEU	A	985	0.747	-14.945	11.571	1.00	25.69
1301	CA	LEU	A	985	1.332	-16.155	11.007	1.00	25.31
1302	C	LEU	A	985	1.351	-16.09	9.482	1.00	25.39
1303	O	LEU	A	985	0.711	-15.234	8.883	1.00	25.35
1304	CB	LEU	A	985	0.534	-17.388	11.447	1.00	25.09
1305	CG	LEU	A	985	0.257	-17.558	12.945	1.00	24.58
1306	CD1	LEU	A	985	-0.301	-18.96	13.166	1.00	23.64
1307	CD2	LEU	A	985	1.542	-17.352	13.766	1.00	21.92
1308	N	SER	A	986	2.104	-16.99	8.859	1.00	25.22
1309	CA	SER	A	986	2.162	-17.05	7.408	1.00	25.44
1310	C	SER	A	986	1.298	-18.212	6.956	1.00	25.87
1311	O	SER	A	986	0.933	-19.083	7.747	1.00	24.46
1312	CB	SER	A	986	3.595	-17.265	6.918	1.00	25.92
1313	OG	SER	A	986	4.401	-16.133	7.182	1.00	28.84
1314	N	ARG	A	987	0.983	-18.234	5.672	1.00	27.01
1315	CA	ARG	A	987	0.152	-19.29	5.129	1.00	27.64
1316	C	ARG	A	987	0.616	-19.578	3.709	1.00	27.3
1317	O	ARG	A	987	0.701	-18.673	2.888	1.00	27.55
1318	CB	ARG	A	987	-1.297	-18.823	5.155	1.00	30.07
1319	CG	ARG	A	987	-2.306	-19.921	5.086	1.00	32.69
1320	CD	ARG	A	987	-3.629	-19.457	5.667	1.00	35.42
1321	NE	ARG	A	987	-4.63	-20.5	5.51	1.00	37.99
1322	CZ	ARG	A	987	-5.091	-20.901	4.333	1.00	38.6
1323	NH1	ARG	A	987	-4.645	-20.335	3.221	1.00	38.95
1324	NH2	ARG	A	987	-5.973	-21.886	4.269	1.00	40.69
1325	N	GLY	A	988	0.933	-20.837	3.432	1.00	27.02

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TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

1326	CA	GLY	A	988	1.406	-21.21	2.114	1.00	27.19
1327	C	GLY	A	988	2.354	-22.391	2.196	1.00	28.07
1328	O	GLY	A	988	2.43	-23.056	3.227	1.00	28.15
1329	N	GLN	A	989	3.084	-22.645	1.118	1.00	28.03
1330	CA	GLN	A	989	4.023	-23.758	1.066	1.00	29.14
1331	C	GLN	A	989	5.342	-23.407	1.751	1.00	28.76
1332	O	GLN	A	989	5.927	-24.226	2.464	1.00	26.52
1333	CB	GLN	A	989	4.31	-24.143	-0.394	1.00	31.54
1334	CG	GLN	A	989	4.944	-25.515	-0.55	1.00	35.77
1335	CD	GLN	A	989	5.56	-25.741	-1.919	1.00	39.85
1336	OE1	GLN	A	989	5.781	-26.884	-2.33	1.00	43.32
1337	NE2	GLN	A	989	5.86	-24.656	-2.626	1.00	40.8
1338	N	GLU	A	990	5.809	-22.186	1.507	1.00	28.69
1339	CA	GLU	A	990	7.06	-21.708	2.079	1.00	28.9
1340	C	GLU	A	990	7.038	-20.19	2.114	1.00	29.03
1341	O	GLU	A	990	6.395	-19.548	1.286	1.00	28.59
1342	CB	GLU	A	990	8.251	-22.19	1.241	1.00	28.73
1343	CG	GLU	A	990	9.615	-21.807	1.798	1.00	30.81
1344	CD	GLU	A	990	10.764	-22.425	1.012	1.00	33.25
1345	OE1	GLU	A	990	10.951	-22.068	-0.167	1.00	34.96
1346	OE2	GLU	A	990	11.483	-23.277	1.569	1.00	34.92
1347	N	VAL	A	991	7.735	-19.618	3.085	1.00	28.74
1348	CA	VAL	A	991	7.792	-18.177	3.201	1.00	29.01
1349	C	VAL	A	991	9.221	-17.733	3.484	1.00	29.98
1350	O	VAL	A	991	9.929	-18.345	4.282	1.00	31.59
1351	CB	VAL	A	991	6.862	-17.669	4.333	1.00	28.66
1352	CG1	VAL	A	991	7.305	-18.24	5.67	1.00	27.53
1353	CG2	VAL	A	991	6.868	-16.146	4.371	1.00	28.65
1354	N	TYR	A	992	9.646	-16.678	2.804	1.00	30.62
1355	CA	TYR	A	992	10.974	-16.118	2.996	1.00	31.06
1356	C	TYR	A	992	10.804	-14.811	3.765	1.00	32.17
1357	O	TYR	A	992	9.999	-13.963	3.378	1.00	31.8
1358	CB	TYR	A	992	11.631	-15.832	1.647	1.00	30.62
1359	CG	TYR	A	992	12.794	-14.863	1.728	1.00	31.51
1360	CD1	TYR	A	992	14.078	-15.3	2.06	1.00	32.53
1361	CD2	TYR	A	992	12.601	-13.5	1.499	1.00	31
1362	CE1	TYR	A	992	15.146	-14.397	2.161	1.00	33.87
1363	CE2	TYR	A	992	13.653	-12.592	1.599	1.00	32.47
1364	CZ	TYR	A	992	14.921	-13.044	1.928	1.00	33.89

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

1365	OH	TYR	A	992	15.956	-12.143	2.026	1.00	36.67
1366	N	VAL	A	993	11.543	-14.656	4.858	1.00	33.76
1367	CA	VAL	A	993	11.476	-13.436	5.662	1.00	36.31
1368	C	VAL	A	993	12.912	-12.958	5.895	1.00	38.55
1369	O	VAL	A	993	13.664	-13.572	6.65	1.00	38.2
1370	CB	VAL	A	993	10.774	-13.693	7.011	1.00	35.88
1371	CG1	VAL	A	993	10.586	-12.383	7.759	1.00	36.09
1372	CG2	VAL	A	993	9.422	-14.363	6.773	1.00	35.43
1373	N	LYS	A	994	13.272	-11.858	5.237	1.00	41.26
1374	CA	LYS	A	994	14.619	-11.288	5.297	1.00	45.23
1375	C	LYS	A	994	15.372	-11.334	6.625	1.00	47.16
1376	O	LYS	A	994	16.406	-12.009	6.72	1.00	47.64
1377	CB	LYS	A	994	14.602	-9.848	4.772	1.00	45.75
1378	CG	LYS	A	994	15.997	-9.291	4.519	1.00	47.13
1379	CD	LYS	A	994	16	-8.249	3.405	1.00	49.06
1380	CE	LYS	A	994	17.423	-7.915	2.979	1.00	50.53
1381	NZ	LYS	A	994	17.455	-6.923	1.862	1.00	51.78
1382	N	ALA	A	995	14.863	-10.621	7.627	1.00	49.13
1383	CA	ALA	A	995	15.459	-10.544	8.97	1.00	53
1384	CB	ALA	A	995	16.876	-11.157	9.002	1.00	51.99
1385	C	ALA	A	995	15.527	-9.09	9.433	1.00	54.38
1386	OT1	ALA	A	995	14.913	-8.778	10.48	1.00	55.53
1387	OT2	ALA	A	995	16.197	-8.286	8.741	1.00	55.74
1388	N	LEU	A	0	15.823	-11.681	16.249	1.00	44.94
1389	CA	LEU	A	0	15.702	-12.994	15.545	1.00	45.05
1390	C	LEU	A	0	15.846	-14.163	16.54	1.00	44.05
1391	O	LEU	A	0	16.834	-14.245	17.278	1.00	44.99
1392	CB	LEU	A	0	16.775	-13.095	14.455	1.00	45.89
1393	CG	LEU	A	0	16.41	-13.896	13.201	1.00	46.91
1394	CD1	LEU	A	0	15.251	-13.21	12.484	1.00	46.88
1395	CD2	LEU	A	0	17.616	-13.998	12.274	1.00	46.64
1396	N	PRO	A	1	14.858	-15.082	16.568	1.00	42.19
1397	CA	PRO	A	1	14.855	-16.248	17.464	1.00	39.07
1398	C	PRO	A	1	15.793	-17.351	16.97	1.00	36.15
1399	O	PRO	A	1	15.382	-18.49	16.745	1.00	34.51
1400	CB	PRO	A	1	13.395	-16.678	17.445	1.00	40.2
1401	CG	PRO	A	1	13.029	-16.444	16.003	1.00	41.49
1402	CD	PRO	A	1	13.66	-15.087	15.703	1.00	41.9
1403	N	VAL	A	2	17.056	-16.986	16.805	1.00	32.98

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

1404	CA	VAL	A	2	18.092	-17.889	16.334	1.00	30.8
1405	C	VAL	A	2	18.103	-19.264	16.999	1.00	29.41
1406	O	VAL	A	2	18.319	-20.281	16.341	1.00	28.83
1407	CB	VAL	A	2	19.485	-17.24	16.537	1.00	30.96
1408	CG1	VAL	A	2	20.59	-18.252	16.263	1.00	29.92
1409	CG2	VAL	A	2	19.618	-16.018	15.634	1.00	29.52
1410	N	ARG	A	3	17.861	-19.291	18.301	1.00	28.39
1411	CA	ARG	A	3	17.902	-20.534	19.058	1.00	27.72
1412	C	ARG	A	3	16.777	-21.542	18.775	1.00	26.09
1413	O	ARG	A	3	16.827	-22.679	19.244	1.00	25.36
1414	CB	ARG	A	3	17.987	-20.184	20.549	1.00	30.07
1415	CG	ARG	A	3	19.063	-19.117	20.822	1.00	33.04
1416	CD	ARG	A	3	19.033	-18.567	22.245	1.00	34.74
1417	NE	ARG	A	3	20.048	-19.195	23.078	1.00	39.08
1418	CZ	ARG	A	3	21.325	-18.828	23.118	1.00	38.72
1419	NH1	ARG	A	3	21.761	-17.817	22.381	1.00	39.28
1420	NH2	ARG	A	3	22.173	-19.497	23.881	1.00	40.7
1421	N	TRP	A	4	15.785	-21.137	17.988	1.00	24.26
1422	CA	TRP	A	4	14.665	-22.014	17.646	1.00	24.64
1423	C	TRP	A	4	14.615	-22.288	16.135	1.00	25.26
1424	O	TRP	A	4	13.865	-23.146	15.666	1.00	25.68
1425	CB	TRP	A	4	13.345	-21.37	18.091	1.00	24.11
1426	CG	TRP	A	4	13.058	-21.469	19.567	1.00	24.56
1427	CD1	TRP	A	4	12.251	-22.385	20.186	1.00	23.83
1428	CD2	TRP	A	4	13.595	-20.637	20.607	1.00	23.47
1429	NE1	TRP	A	4	12.256	-22.176	21.55	1.00	24.3
1430	CE2	TRP	A	4	13.07	-21.109	21.833	1.00	23.59
1431	CE3	TRP	A	4	14.468	-19.54	20.623	1.00	24.81
1432	CZ2	TRP	A	4	13.392	-20.522	23.064	1.00	23.28
1433	CZ3	TRP	A	4	14.79	-18.954	21.851	1.00	24.66
1434	CH2	TRP	A	4	14.249	-19.45	23.054	1.00	24.47
1435	N	MET	A	5	15.433	-21.561	15.387	1.00	24.75
1436	CA	MET	A	5	15.471	-21.674	13.937	1.00	25.45
1437	C	MET	A	5	16.165	-22.895	13.355	1.00	26.24
1438	O	MET	A	5	17.264	-23.264	13.77	1.00	26.18
1439	CB	MET	A	5	16.098	-20.403	13.357	1.00	26.67
1440	CG	MET	A	5	15.221	-19.178	13.534	1.00	26.85
1441	SD	MET	A	5	16.058	-17.619	13.232	1.00	30.27
1442	CE	MET	A	5	16.578	-17.826	11.497	1.00	26.28

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

1443	N	ALA	A	6	15.51	-23.513	12.375	1.00	25.86
1444	CA	ALA	A	6	16.048	-24.682	11.696	1.00	26.26
1445	C	ALA	A	6	17.237	-24.264	10.826	1.00	27.11
1446	O	ALA	A	6	17.348	-23.104	10.431	1.00	26.38
1447	CB	ALA	A	6	14.969	-25.321	10.831	1.00	25.38
1448	N	ILE	A	7	18.118	-25.211	10.523	1.00	28.06
1449	CA	ILE	A	7	19.291	-24.918	9.704	1.00	30.33
1450	C	ILE	A	7	18.966	-24.199	8.39	1.00	30.29
1451	O	ILE	A	7	19.66	-23.251	8.014	1.00	30.72
1452	CB	ILE	A	7	20.091	-26.209	9.406	1.00	31.52
1453	CG1	ILE	A	7	20.846	-26.633	10.671	1.00	33.3
1454	CG2	ILE	A	7	21.064	-25.977	8.25	1.00	33.25
1455	CD1	ILE	A	7	21.656	-27.908	10.527	1.00	36.49
1456	N	GLU	A	8	17.916	-24.634	7.694	1.00	29.58
1457	CA	GLU	A	8	17.556	-23.984	6.436	1.00	29.55
1458	C	GLU	A	8	17.147	-22.529	6.667	1.00	28.47
1459	O	GLU	A	8	17.375	-21.677	5.806	1.00	28.12
1460	CB	GLU	A	8	16.426	-24.744	5.714	1.00	29.51
1461	CG	GLU	A	8	15.121	-24.842	6.484	1.00	29.32
1462	CD	GLU	A	8	14.984	-26.144	7.255	1.00	29.66
1463	OE1	GLU	A	8	16.004	-26.652	7.772	1.00	28.68
1464	OE2	GLU	A	8	13.846	-26.649	7.358	1.00	29.34
1465	N	SER	A	9	16.543	-22.245	7.823	1.00	27.21
1466	CA	SER	A	9	16.126	-20.878	8.151	1.00	26.35
1467	C	SER	A	9	17.349	-20.008	8.44	1.00	26.56
1468	O	SER	A	9	17.422	-18.853	8.02	1.00	25.43
1469	CB	SER	A	9	15.203	-20.869	9.378	1.00	27.02
1470	OG	SER	A	9	13.954	-21.495	9.12	1.00	28.67
1471	N	LEU	A	10	18.302	-20.566	9.18	1.00	27.26
1472	CA	LEU	A	10	19.525	-19.852	9.511	1.00	27.38
1473	C	LEU	A	10	20.281	-19.547	8.217	1.00	28.06
1474	O	LEU	A	10	20.779	-18.441	8.032	1.00	27.98
1475	CB	LEU	A	10	20.4	-20.701	10.448	1.00	26.81
1476	CG	LEU	A	10	19.863	-20.974	11.862	1.00	26.11
1477	CD1	LEU	A	10	20.709	-22.026	12.548	1.00	25.38
1478	CD2	LEU	A	10	19.855	-19.683	12.667	1.00	26.26
1479	N	ASN	A	11	20.344	-20.525	7.318	1.00	29.13
1480	CA	ASN	A	11	21.048	-20.346	6.047	1.00	31.46
1481	C	ASN	A	11	20.358	-19.474	4.997	1.00	31.52

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

1482	O	ASN	A	11	20.991	-18.601	4.407	1.00	31.98
1483	CB	ASN	A	11	21.341	-21.7	5.387	1.00	32.76
1484	CG	ASN	A	11	22.39	-22.5	6.123	1.00	33.7
1485	OD1	ASN	A	11	23.227	-21.944	6.828	1.00	35.6
1486	ND2	ASN	A	11	22.364	-23.813	5.944	1.00	34.91
1487	N	TYR	A	12	19.066	-19.696	4.768	1.00	31.68
1488	CA	TYR	A	12	18.362	-18.966	3.719	1.00	31.16
1489	C	TYR	A	12	17.148	-18.132	4.107	1.00	31.38
1490	O	TYR	A	12	16.472	-17.578	3.239	1.00	31.22
1491	CB	TYR	A	12	17.956	-19.957	2.635	1.00	32.4
1492	CG	TYR	A	12	19.079	-20.871	2.198	1.00	34.24
1493	CD1	TYR	A	12	19.018	-22.241	2.436	1.00	34.45
1494	CD2	TYR	A	12	20.197	-20.366	1.529	1.00	35.19
1495	CE1	TYR	A	12	20.04	-23.091	2.019	1.00	35.92
1496	CE2	TYR	A	12	21.224	-21.207	1.104	1.00	35.93
1497	CZ	TYR	A	12	21.137	-22.568	1.351	1.00	36.74
1498	OH	TYR	A	12	22.143	-23.411	0.927	1.00	38.87
1499	N	SER	A	13	16.863	-18.04	5.398	1.00	30.82
1500	CA	SER	A	13	15.723	-17.26	5.863	1.00	30.92
1501	C	SER	A	13	14.386	-17.749	5.307	1.00	30.78
1502	O	SER	A	13	13.482	-16.945	5.049	1.00	31.27
1503	CB	SER	A	13	15.907	-15.783	5.501	1.00	31.67
1504	OG	SER	A	13	17.16	-15.308	5.963	1.00	33.52
1505	N	VAL	A	14	14.259	-19.059	5.116	1.00	29.84
1506	CA	VAL	A	14	13.014	-19.627	4.616	1.00	28.58
1507	C	VAL	A	14	12.332	-20.406	5.729	1.00	28.87
1508	O	VAL	A	14	12.998	-21.008	6.573	1.00	29.24
1509	CB	VAL	A	14	13.25	-20.569	3.414	1.00	28.49
1510	CG1	VAL	A	14	13.744	-19.772	2.213	1.00	27.83
1511	CG2	VAL	A	14	14.247	-21.644	3.786	1.00	28.21
1512	N	TYR	A	15	11.003	-20.387	5.731	1.00	27.76
1513	CA	TYR	A	15	10.232	-21.088	6.745	1.00	25.92
1514	C	TYR	A	15	9.164	-21.989	6.129	1.00	25.9
1515	O	TYR	A	15	8.458	-21.595	5.196	1.00	25.1
1516	CB	TYR	A	15	9.569	-20.083	7.694	1.00	26.37
1517	CG	TYR	A	15	10.549	-19.181	8.408	1.00	26.88
1518	CD1	TYR	A	15	11.101	-18.073	7.766	1.00	26.47
1519	CD2	TYR	A	15	10.96	-19.463	9.715	1.00	26.74
1520	CE1	TYR	A	15	12.045	-17.264	8.405	1.00	28.02

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

1521	CE2	TYR	A	15	11.903	-18.666	10.361	1.00	26.77
1522	CZ	TYR	A	15	12.442	-17.572	9.701	1.00	27.41
1523	OH	TYR	A	15	13.392	-16.805	10.327	1.00	29.1
1524	N	THR	A	16	9.053	-23.2	6.665	1.00	24.61
1525	CA	THR	A	16	8.078	-24.176	6.189	1.00	24.76
1526	C	THR	A	16	7.494	-24.883	7.396	1.00	24.89
1527	O	THR	A	16	7.928	-24.661	8.53	1.00	24.23
1528	CB	THR	A	16	8.729	-25.261	5.32	1.00	23.97
1529	OG1	THR	A	16	9.552	-26.092	6.147	1.00	22.98
1530	CG2	THR	A	16	9.585	-24.64	4.229	1.00	25.04
1531	N	THR	A	17	6.515	-25.743	7.155	1.00	25.94
1532	CA	THR	A	17	5.918	-26.493	8.244	1.00	27.51
1533	C	THR	A	17	6.994	-27.457	8.785	1.00	27.58
1534	O	THR	A	17	6.944	-27.863	9.939	1.00	27.85
1535	CB	THR	A	17	4.666	-27.259	7.764	1.00	28.08
1536	OG1	THR	A	17	3.927	-27.717	8.898	1.00	33.09
1537	CG2	THR	A	17	5.054	-28.453	6.916	1.00	29.54
1538	N	ASN	A	18	7.976	-27.797	7.949	1.00	28.25
1539	CA	ASN	A	18	9.074	-28.677	8.363	1.00	28.81
1540	C	ASN	A	18	9.984	-27.953	9.356	1.00	28.7
1541	O	ASN	A	18	10.486	-28.562	10.303	1.00	30.52
1542	CB	ASN	A	18	9.934	-29.117	7.169	1.00	31.08
1543	CG	ASN	A	18	9.317	-30.263	6.377	1.00	33.79
1544	OD1	ASN	A	18	8.669	-31.148	6.936	1.00	35.23
1545	ND2	ASN	A	18	9.547	-30.264	5.07	1.00	33.61
1546	N	SER	A	19	10.215	-26.661	9.128	1.00	26.72
1547	CA	SER	A	19	11.061	-25.891	10.028	1.00	25.19
1548	C	SER	A	19	10.298	-25.602	11.32	1.00	24.68
1549	O	SER	A	19	10.903	-25.386	12.368	1.00	25.4
1550	CB	SER	A	19	11.535	-24.589	9.362	1.00	25.44
1551	OG	SER	A	19	10.471	-23.693	9.083	1.00	25.41
1552	N	ASP	A	20	8.968	-25.601	11.252	1.00	23.85
1553	CA	ASP	A	20	8.171	-25.381	12.454	1.00	23.11
1554	C	ASP	A	20	8.387	-26.596	13.356	1.00	22.97
1555	O	ASP	A	20	8.386	-26.481	14.581	1.00	22.69
1556	CB	ASP	A	20	6.677	-25.262	12.134	1.00	23.1
1557	CG	ASP	A	20	6.237	-23.831	11.82	1.00	23.28
1558	OD1	ASP	A	20	6.969	-22.866	12.144	1.00	22.85
1559	OD2	ASP	A	20	5.132	-23.677	11.258	1.00	21.69

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

1560	N	VAL	A	21	8.569	-27.76	12.738	1.00	21.52
1561	CA	VAL	A	21	8.797	-28.998	13.481	1.00	21.21
1562	C	VAL	A	21	10.154	-28.961	14.206	1.00	21.54
1563	O	VAL	A	21	10.297	-29.507	15.303	1.00	21.32
1564	CB	VAL	A	21	8.705	-30.226	12.534	1.00	21.27
1565	CG1	VAL	A	21	9.348	-31.462	13.172	1.00	20.42
1566	CG2	VAL	A	21	7.223	-30.511	12.229	1.00	20.66
1567	N	TRP	A	22	11.144	-28.313	13.599	1.00	20.43
1568	CA	TRP	A	22	12.449	-28.189	14.236	1.00	21.32
1569	C	TRP	A	22	12.241	-27.31	15.468	1.00	21.43
1570	O	TRP	A	22	12.7	-27.639	16.555	1.00	22.62
1571	CB	TRP	A	22	13.453	-27.532	13.283	1.00	21.78
1572	CG	TRP	A	22	14.791	-27.221	13.902	1.00	22.26
1573	CD1	TRP	A	22	15.039	-26.363	14.94	1.00	21.88
1574	CD2	TRP	A	22	16.067	-27.749	13.506	1.00	22.33
1575	NE1	TRP	A	22	16.385	-26.324	15.21	1.00	23.01
1576	CE2	TRP	A	22	17.039	-27.167	14.349	1.00	23.26
1577	CE3	TRP	A	22	16.479	-28.659	12.52	1.00	22.84
1578	CZ2	TRP	A	22	18.41	-27.46	14.235	1.00	23.26
1579	CZ3	TRP	A	22	17.841	-28.952	12.406	1.00	25.15
1580	CH2	TRP	A	22	18.789	-28.353	13.265	1.00	24.32
1581	N	SER	A	23	11.535	-26.197	15.296	1.00	21.21
1582	CA	SER	A	23	11.27	-25.293	16.412	1.00	21.11
1583	C	SER	A	23	10.508	-26.017	17.511	1.00	21.09
1584	O	SER	A	23	10.779	-25.816	18.697	1.00	21.72
1585	CB	SER	A	23	10.473	-24.076	15.943	1.00	20.67
1586	OG	SER	A	23	11.2	-23.359	14.963	1.00	22.95
1587	N	TYR	A	24	9.557	-26.864	17.122	1.00	20.16
1588	CA	TYR	A	24	8.784	-27.621	18.103	1.00	19.18
1589	C	TYR	A	24	9.731	-28.493	18.947	1.00	18.69
1590	O	TYR	A	24	9.515	-28.695	20.147	1.00	18.05
1591	CB	TYR	A	24	7.755	-28.524	17.415	1.00	17.82
1592	CG	TYR	A	24	7.011	-29.378	18.414	1.00	19.47
1593	CD1	TYR	A	24	5.915	-28.872	19.107	1.00	20.09
1594	CD2	TYR	A	24	7.465	-30.659	18.744	1.00	18.49
1595	CE1	TYR	A	24	5.289	-29.614	20.113	1.00	20.36
1596	CE2	TYR	A	24	6.847	-31.408	19.747	1.00	18.17
1597	CZ	TYR	A	24	5.76	-30.874	20.428	1.00	19.84
1598	OH	TYR	A	24	5.155	-31.588	21.441	1.00	21.09



TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

1599	N	GLY	A	25	10.77	-29.022	18.309	1.00	18.82
1600	CA	GLY	A	25	11.729	-29.845	19.031	1.00	18.56
1601	C	GLY	A	25	12.373	-29.058	20.162	1.00	19.38
1602	O	GLY	A	25	12.506	-29.556	21.286	1.00	18.95
1603	N	VAL	A	26	12.766	-27.821	19.864	1.00	17.72
1604	CA	VAL	A	26	13.39	-26.962	20.852	1.00	18.54
1605	C	VAL	A	26	12.382	-26.618	21.952	1.00	20.12
1606	O	VAL	A	26	12.727	-26.547	23.133	1.00	21.63
1607	CB	VAL	A	26	13.908	-25.662	20.199	1.00	18.45
1608	CG1	VAL	A	26	14.666	-24.832	21.228	1.00	17.61
1609	CG2	VAL	A	26	14.805	-25.996	19.007	1.00	15.59
1610	N	LEU	A	27	11.133	-26.401	21.56	1.00	20.23
1611	CA	LEU	A	27	10.077	-26.087	22.513	1.00	19.59
1612	C	LEU	A	27	9.879	-27.283	23.459	1.00	19.12
1613	O	LEU	A	27	9.67	-27.112	24.663	1.00	19.49
1614	CB	LEU	A	27	8.773	-25.769	21.759	1.00	19.74
1615	CG	LEU	A	27	7.566	-25.36	22.608	1.00	20.12
1616	CD1	LEU	A	27	6.578	-24.546	21.776	1.00	22.69
1617	CD2	LEU	A	27	6.91	-26.597	23.158	1.00	21.35
1618	N	LEU	A	28	9.931	-28.491	22.913	1.00	18.62
1619	CA	LEU	A	28	9.782	-29.691	23.736	1.00	19.48
1620	C	LEU	A	28	10.946	-29.723	24.725	1.00	20.51
1621	O	LEU	A	28	10.803	-30.155	25.871	1.00	20.18
1622	CB	LEU	A	28	9.801	-30.959	22.859	1.00	18.17
1623	CG	LEU	A	28	9.747	-32.314	23.59	1.00	18.55
1624	CD1	LEU	A	28	8.555	-32.36	24.537	1.00	17.32
1625	CD2	LEU	A	28	9.667	-33.449	22.578	1.00	19.07
1626	N	TRP	A	29	12.103	-29.261	24.263	1.00	20.77
1627	CA	TRP	A	29	13.293	-29.211	25.099	1.00	22.17
1628	C	TRP	A	29	13.051	-28.195	26.224	1.00	21.69
1629	O	TRP	A	29	13.483	-28.402	27.353	1.00	22.1
1630	CB	TRP	A	29	14.508	-28.801	24.258	1.00	21.93
1631	CG	TRP	A	29	15.827	-28.932	24.97	1.00	24.92
1632	CD1	TRP	A	29	16.676	-30.007	24.946	1.00	25.6
1633	CD2	TRP	A	29	16.457	-27.942	25.792	1.00	24.49
1634	NE1	TRP	A	29	17.797	-29.743	25.699	1.00	26.26
1635	CE2	TRP	A	29	17.687	-28.484	26.23	1.00	25.93
1636	CE3	TRP	A	29	16.101	-26.65	26.201	1.00	24.05
1637	CZ2	TRP	A	29	18.567	-27.775	27.057	1.00	25.58

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

1638	CZ3	TRP	A	29	16.976	-25.945	27.021	1.00	25.49
1639	CH2	TRP	A	29	18.196	-26.509	27.441	1.00	24.3
1640	N	GLU	A	30	12.351	-27.104	25.913	1.00	21.23
1641	CA	GLU	A	30	12.05	-26.09	26.925	1.00	21.39
1642	C	GLU	A	30	11.133	-26.648	28.003	1.00	21.46
1643	O	GLU	A	30	11.315	-26.372	29.184	1.00	21.7
1644	CB	GLU	A	30	11.355	-24.877	26.311	1.00	20.7
1645	CG	GLU	A	30	12.198	-24.067	25.359	1.00	21.19
1646	CD	GLU	A	30	11.469	-22.829	24.905	1.00	20.45
1647	OE1	GLU	A	30	11.483	-21.821	25.647	1.00	21.52
1648	OE2	GLU	A	30	10.864	-22.874	23.816	1.00	18.94
1649	N	ILE	A	31	10.126	-27.407	27.583	1.00	21.79
1650	CA	ILE	A	31	9.182	-27.997	28.521	1.00	21.71
1651	C	ILE	A	31	9.903	-28.966	29.448	1.00	21.91
1652	O	ILE	A	31	9.737	-28.917	30.668	1.00	22.5
1653	CB	ILE	A	31	8.047	-28.75	27.772	1.00	20.54
1654	CG1	ILE	A	31	7.117	-27.734	27.1	1.00	20.51
1655	CG2	ILE	A	31	7.273	-29.648	28.742	1.00	19.34
1656	CD1	ILE	A	31	6.054	-28.363	26.235	1.00	23.1
1657	N	VAL	A	32	10.715	-29.835	28.856	1.00	22.06
1658	CA	VAL	A	32	11.451	-30.838	29.607	1.00	21.87
1659	C	VAL	A	32	12.428	-30.224	30.608	1.00	22.44
1660	O	VAL	A	32	12.557	-30.713	31.727	1.00	21.92
1661	CB	VAL	A	32	12.223	-31.79	28.65	1.00	22.28
1662	CG1	VAL	A	32	13.121	-32.743	29.457	1.00	21.44
1663	CG2	VAL	A	32	11.233	-32.593	27.809	1.00	20.88
1664	N	SER	A	33	13.11	-29.154	30.209	1.00	23.08
1665	CA	SER	A	33	14.075	-28.507	31.091	1.00	23.23
1666	C	SER	A	33	13.433	-27.477	32.014	1.00	23.58
1667	O	SER	A	33	14.131	-26.721	32.683	1.00	23.31
1668	CB	SER	A	33	15.175	-27.838	30.272	1.00	22.63
1669	OG	SER	A	33	14.658	-26.738	29.556	1.00	25.43
1670	N	LEU	A	34	12.106	-27.451	32.055	1.00	22.64
1671	CA	LEU	A	34	11.4	-26.508	32.913	1.00	23.12
1672	C	LEU	A	34	11.712	-25.042	32.598	1.00	23.09
1673	O	LEU	A	34	11.862	-24.217	33.505	1.00	23.33
1674	CB	LEU	A	34	11.72	-26.804	34.381	1.00	23.35
1675	CG	LEU	A	34	11.35	-28.223	34.831	1.00	24.59
1676	CD1	LEU	A	34	11.902	-28.488	36.232	1.00	23.47

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TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

1677	CD2	LEU	A	34	9.832	-28.385	34.798	1.00	21.94
1678	N	GLY	A	35	11.816	-24.717	31.313	1.00	23.86
1679	CA	GLY	A	35	12.073	-23.341	30.923	1.00	23.55
1680	C	GLY	A	35	13.521	-22.92	30.778	1.00	23.41
1681	O	GLY	A	35	13.832	-21.731	30.832	1.00	24.56
1682	N	GLY	A	36	14.416	-23.877	30.59	1.00	24.03
1683	CA	GLY	A	36	15.813	-23.519	30.426	1.00	24.92
1684	C	GLY	A	36	16.063	-22.839	29.09	1.00	25.76
1685	O	GLY	A	36	15.314	-23.026	28.13	1.00	26.38
1686	N	THR	A	37	17.114	-22.033	29.028	1.00	26.19
1687	CA	THR	A	37	17.465	-21.342	27.801	1.00	25.67
1688	C	THR	A	37	18.197	-22.287	26.859	1.00	26.03
1689	O	THR	A	37	19.228	-22.851	27.211	1.00	27.37
1690	CB	THR	A	37	18.379	-20.144	28.084	1.00	26.42
1691	OG1	THR	A	37	17.701	-19.22	28.942	1.00	26.93
1692	CG2	THR	A	37	18.758	-19.447	26.793	1.00	25.26
1693	N	PRO	A	38	17.66	-22.488	25.65	1.00	25.71
1694	CA	PRO	A	38	18.282	-23.373	24.66	1.00	25.3
1695	C	PRO	A	38	19.717	-22.931	24.351	1.00	24.89
1696	O	PRO	A	38	19.962	-21.762	24.069	1.00	23.17
1697	CB	PRO	A	38	17.369	-23.218	23.442	1.00	25.48
1698	CG	PRO	A	38	16.032	-22.935	24.055	1.00	25.45
1699	CD	PRO	A	38	16.374	-21.962	25.158	1.00	25.51
1700	N	TYR	A	39	20.657	-23.868	24.401	1.00	26
1701	CA	TYR	A	39	22.061	-23.568	24.12	1.00	28.26
1702	C	TYR	A	39	22.599	-22.504	25.098	1.00	29.62
1703	O	TYR	A	39	23.419	-21.665	24.719	1.00	27.3
1704	CB	TYR	A	39	22.218	-23.05	22.685	1.00	26.53
1705	CG	TYR	A	39	21.55	-23.889	21.609	1.00	27.39
1706	CD1	TYR	A	39	22.118	-25.085	21.169	1.00	26.72
1707	CD2	TYR	A	39	20.359	-23.469	21.013	1.00	26.56
1708	CE1	TYR	A	39	21.522	-25.843	20.157	1.00	25.39
1709	CE2	TYR	A	39	19.753	-24.215	20.008	1.00	26.67
1710	CZ	TYR	A	39	20.34	-25.399	19.581	1.00	26.98
1711	OH	TYR	A	39	19.757	-26.121	18.563	1.00	24.88
1712	N	CYS	A	40	22.126	-22.539	26.344	1.00	32.15
1713	CA	CYS	A	40	22.562	-21.576	27.353	1.00	35.57
1714	C	CYS	A	40	24.085	-21.548	27.406	1.00	36.1
1715	O	CYS	A	40	24.72	-22.561	27.686	1.00	35.71

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

1716	CB	CYS	A	40	22.008	-21.952	28.733	1.00	36.51
1717	SG	CYS	A	40	22.219	-20.661	30.001	1.00	41.87
1718	N	GLY	A	41	24.664	-20.385	27.129	1.00	37.79
1719	CA	GLY	A	41	26.109	-20.265	27.142	1.00	40.54
1720	C	GLY	A	41	26.689	-19.979	25.769	1.00	41.96
1721	O	GLY	A	41	27.57	-19.126	25.628	1.00	43.19
1722	N	MET	A	42	26.204	-20.69	24.755	1.00	42.58
1723	CA	MET	A	42	26.674	-20.498	23.386	1.00	43.31
1724	C	MET	A	42	26.101	-19.207	22.81	1.00	43.61
1725	O	MET	A	42	24.988	-18.807	23.149	1.00	44.4
1726	CB	MET	A	42	26.247	-21.679	22.512	1.00	44.23
1727	CG	MET	A	42	26.852	-23.001	22.927	1.00	45.13
1728	SD	MET	A	42	26.19	-24.391	22.001	1.00	46.84
1729	CE	MET	A	42	27.211	-24.333	20.513	1.00	47.48
1730	N	THR	A	43	26.863	-18.552	21.943	1.00	43.45
1731	CA	THR	A	43	26.398	-17.313	21.33	1.00	43.45
1732	C	THR	A	43	25.701	-17.643	20.015	1.00	43.62
1733	O	THR	A	43	25.875	-18.733	19.467	1.00	43.14
1734	CB	THR	A	43	27.565	-16.358	21.025	1.00	43.23
1735	OG1	THR	A	43	28.329	-16.873	19.927	1.00	43.44
1736	CG2	THR	A	43	28.473	-16.22	22.244	1.00	42.98
1737	N	CYS	A	44	24.912	-16.701	19.514	1.00	43.9
1738	CA	CYS	A	44	24.21	-16.902	18.258	1.00	44.16
1739	C	CYS	A	44	25.216	-17.199	17.149	1.00	43.96
1740	O	CYS	A	44	24.959	-18.02	16.276	1.00	43.73
1741	CB	CYS	A	44	23.376	-15.663	17.914	1.00	44.99
1742	SG	CYS	A	44	21.95	-15.38	19.026	1.00	49.02
1743	N	ALA	A	45	26.369	-16.542	17.195	1.00	44.46
1744	CA	ALA	A	45	27.403	-16.753	16.186	1.00	45.37
1745	C	ALA	A	45	27.868	-18.205	16.188	1.00	45.57
1746	O	ALA	A	45	28.068	-18.807	15.132	1.00	45.81
1747	CB	ALA	A	45	28.585	-15.822	16.443	1.00	45.27
1748	N	GLU	A	46	28.044	-18.767	17.377	1.00	46.31
1749	CA	GLU	A	46	28.474	-20.155	17.493	1.00	46.87
1750	C	GLU	A	46	27.439	-21.096	16.889	1.00	46.51
1751	O	GLU	A	46	27.79	-22.101	16.267	1.00	46.43
1752	CB	GLU	A	46	28.693	-20.525	18.956	1.00	48.35
1753	CG	GLU	A	46	29.926	-19.912	19.578	1.00	50.4
1754	CD	GLU	A	46	30.08	-20.309	21.028	1.00	52.23

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

1755	OE1	GLU	A	46	29.323	-19.784	21.873	1.00	52.77
1756	OE2	GLU	A	46	30.948	-21.159	21.318	1.00	53.92
1757	N	LEU	A	47	26.163	-20.769	17.072	1.00	45.34
1758	CA	LEU	A	47	25.097	-21.606	16.539	1.00	44.64
1759	C	LEU	A	47	25.128	-21.683	15.014	1.00	44.39
1760	O	LEU	A	47	25.031	-22.774	14.45	1.00	44.43
1761	CB	LEU	A	47	23.73	-21.103	17.018	1.00	42.96
1762	CG	LEU	A	47	23.466	-21.287	18.515	1.00	42.26
1763	CD1	LEU	A	47	22.117	-20.694	18.882	1.00	40.97
1764	CD2	LEU	A	47	23.518	-22.769	18.863	1.00	41.95
1765	N	TYR	A	48	25.267	-20.539	14.345	1.00	44.17
1766	CA	TYR	A	48	25.308	-20.538	12.882	1.00	44.42
1767	C	TYR	A	48	26.439	-21.425	12.38	1.00	44.95
1768	O	TYR	A	48	26.378	-21.964	11.279	1.00	46.19
1769	CB	TYR	A	48	25.509	-19.122	12.322	1.00	42.99
1770	CG	TYR	A	48	24.265	-18.258	12.269	1.00	42.15
1771	CD1	TYR	A	48	23.845	-17.528	13.383	1.00	42
1772	CD2	TYR	A	48	23.512	-18.158	11.095	1.00	41.7
1773	CE1	TYR	A	48	22.703	-16.716	13.327	1.00	40.72
1774	CE2	TYR	A	48	22.371	-17.352	11.031	1.00	39.54
1775	CZ	TYR	A	48	21.975	-16.636	12.148	1.00	39.96
1776	OH	TYR	A	48	20.85	-15.846	12.09	1.00	38.43
1777	N	GLU	A	49	27.467	-21.582	13.203	1.00	46.19
1778	CA	GLU	A	49	28.628	-22.382	12.845	1.00	46.88
1779	C	GLU	A	49	28.502	-23.87	13.178	1.00	47.07
1780	O	GLU	A	49	28.659	-24.725	12.302	1.00	46.83
1781	CB	GLU	A	49	29.863	-21.795	13.533	1.00	48.59
1782	CG	GLU	A	49	31.161	-22.552	13.308	1.00	51.87
1783	CD	GLU	A	49	32.354	-21.853	13.953	1.00	54.06
1784	OE1	GLU	A	49	32.335	-21.642	15.188	1.00	53.96
1785	OE2	GLU	A	49	33.312	-21.509	13.222	1.00	55.43
1786	N	LYS	A	50	28.205	-24.177	14.438	1.00	46.34
1787	CA	LYS	A	50	28.105	-25.566	14.884	1.00	45.45
1788	C	LYS	A	50	26.893	-26.394	14.446	1.00	44.62
1789	O	LYS	A	50	27.029	-27.592	14.175	1.00	43.25
1790	CB	LYS	A	50	28.228	-25.623	16.408	1.00	46.27
1791	CG	LYS	A	50	29.627	-25.334	16.925	1.00	47.53
1792	CD	LYS	A	50	29.701	-25.521	18.431	1.00	49.02
1793	CE	LYS	A	50	31.143	-25.649	18.91	1.00	50.62

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

1794	NZ	LYS	A	50	31.984	-24.483	18.513	1.00	51.42
1795	N	LEU	A	51	25.715	-25.779	14.386	1.00	43.57
1796	CA	LEU	A	51	24.518	-26.514	13.993	1.00	43.13
1797	C	LEU	A	51	24.668	-27.19	12.632	1.00	43.55
1798	O	LEU	A	51	24.346	-28.368	12.478	1.00	43.03
1799	CB	LEU	A	51	23.293	-25.593	14.001	1.00	42.44
1800	CG	LEU	A	51	22.877	-25.097	15.39	1.00	43.07
1801	CD1	LEU	A	51	21.683	-24.167	15.272	1.00	44.16
1802	CD2	LEU	A	51	22.537	-26.282	16.281	1.00	42.36
1803	N	PRO	A	52	25.157	-26.455	11.621	1.00	44.31
1804	CA	PRO	A	52	25.317	-27.079	10.304	1.00	44.78
1805	C	PRO	A	52	26.347	-28.211	10.313	1.00	44.93
1806	O	PRO	A	52	26.391	-29.024	9.394	1.00	45.29
1807	CB	PRO	A	52	25.74	-25.908	9.42	1.00	44.67
1808	CG	PRO	A	52	25.027	-24.744	10.06	1.00	44.3
1809	CD	PRO	A	52	25.307	-24.993	11.524	1.00	44.17
1810	N	GLN	A	53	27.174	-28.257	11.353	1.00	45.55
1811	CA	GLN	A	53	28.193	-29.297	11.476	1.00	45.93
1812	C	GLN	A	53	27.621	-30.568	12.093	1.00	44.92
1813	O	GLN	A	53	28.258	-31.62	12.065	1.00	45.09
1814	CB	GLN	A	53	29.358	-28.806	12.336	1.00	47.86
1815	CG	GLN	A	53	30.2	-27.72	11.688	1.00	51.23
1816	CD	GLN	A	53	31.295	-27.21	12.609	1.00	53.32
1817	OE1	GLN	A	53	32.157	-26.434	12.196	1.00	54.44
1818	NE2	GLN	A	53	31.262	-27.643	13.868	1.00	53.93
1819	N	GLY	A	54	26.422	-30.465	12.658	1.00	43.66
1820	CA	GLY	A	54	25.796	-31.624	13.265	1.00	41.68
1821	C	GLY	A	54	25.525	-31.468	14.749	1.00	41.16
1822	O	GLY	A	54	24.939	-32.359	15.368	1.00	41.05
1823	N	TYR	A	55	25.94	-30.343	15.327	1.00	40.11
1824	CA	TYR	A	55	25.722	-30.104	16.751	1.00	39.53
1825	C	TYR	A	55	24.242	-29.95	17.088	1.00	38.2
1826	O	TYR	A	55	23.492	-29.298	16.362	1.00	37.94
1827	CB	TYR	A	55	26.48	-28.855	17.213	1.00	40.94
1828	CG	TYR	A	55	26.319	-28.57	18.694	1.00	43.13
1829	CD1	TYR	A	55	25.241	-27.824	19.169	1.00	43.96
1830	CD2	TYR	A	55	27.217	-29.032	19.625	1.00	44.27
1831	CE1	TYR	A	55	25.057	-27.606	20.534	1.00	45
1832	CE2	TYR	A	55	27.041	-28.883	20.995	1.00	45.39

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

1833	CZ	TYR	A	55	25.959	-28.14	21.442	1.00	45.31
1834	OH	TYR	A	55	25.765	-27.943	22.792	1.00	46.49
1835	N	ARG	A	56	23.827	-30.554	18.196	1.00	36.79
1836	CA	ARG	A	56	22.437	-30.475	18.636	1.00	35.18
1837	C	ARG	A	56	22.35	-30.312	20.153	1.00	34.76
1838	O	ARG	A	56	23.289	-30.652	20.884	1.00	33.68
1839	CB	ARG	A	56	21.677	-31.742	18.229	1.00	33.52
1840	CG	ARG	A	56	21.555	-31.965	16.726	1.00	33.32
1841	CD	ARG	A	56	20.638	-30.939	16.068	1.00	32.44
1842	NE	ARG	A	56	20.404	-31.242	14.658	1.00	31.32
1843	CZ	ARG	A	56	21.222	-30.903	13.666	1.00	30.87
1844	NH1	ARG	A	56	22.339	-30.236	13.923	1.00	30.29
1845	NH2	ARG	A	56	20.923	-31.237	12.416	1.00	30.17
1846	N	LEU	A	57	21.221	-29.782	20.619	1.00	33.41
1847	CA	LEU	A	57	20.992	-29.614	22.049	1.00	32.62
1848	C	LEU	A	57	21.197	-30.965	22.73	1.00	33.05
1849	O	LEU	A	57	20.813	-32.007	22.194	1.00	33.12
1850	CB	LEU	A	57	19.561	-29.147	22.313	1.00	30.44
1851	CG	LEU	A	57	19.197	-27.689	22.045	1.00	30.3
1852	CD1	LEU	A	57	17.68	-27.544	22.043	1.00	28.67
1853	CD2	LEU	A	57	19.834	-26.797	23.113	1.00	28.8
1854	N	GLU	A	58	21.79	-30.945	23.916	1.00	33.68
1855	CA	GLU	A	58	22.034	-32.171	24.661	1.00	35.36
1856	C	GLU	A	58	20.805	-32.57	25.472	1.00	33.87
1857	O	GLU	A	58	19.963	-31.732	25.804	1.00	33.34
1858	CB	GLU	A	58	23.25	-31.987	25.573	1.00	38.11
1859	CG	GLU	A	58	24.539	-31.788	24.785	1.00	43.89
1860	CD	GLU	A	58	25.631	-31.114	25.589	1.00	47.35
1861	OE1	GLU	A	58	26.085	-31.699	26.597	1.00	48.97
1862	OE2	GLU	A	58	26.034	-29.992	25.208	1.00	50.79
1863	N	LYS	A	59	20.709	-33.859	25.78	1.00	32.6
1864	CA	LYS	A	59	19.585	-34.393	26.534	1.00	32.19
1865	C	LYS	A	59	19.517	-33.888	27.966	1.00	31.14
1866	O	LYS	A	59	20.46	-34.048	28.738	1.00	30.61
1867	CB	LYS	A	59	19.638	-35.922	26.56	1.00	32.41
1868	CG	LYS	A	59	18.433	-36.545	27.248	1.00	33.94
1869	CD	LYS	A	59	18.474	-38.06	27.206	1.00	35.83
1870	CE	LYS	A	59	19.521	-38.599	28.153	1.00	37.58
1871	NZ	LYS	A	59	19.584	-40.079	28.094	1.00	40.78

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

1872	N	PRO	A	60	18.391	-33.272	28.342	1.00	30.59
1873	CA	PRO	A	60	18.271	-32.774	29.716	1.00	30.45
1874	C	PRO	A	60	18.511	-33.955	30.663	1.00	30.61
1875	O	PRO	A	60	18.234	-35.1	30.317	1.00	29.49
1876	CB	PRO	A	60	16.838	-32.252	29.77	1.00	30.66
1877	CG	PRO	A	60	16.596	-31.798	28.357	1.00	30.76
1878	CD	PRO	A	60	17.203	-32.928	27.543	1.00	29.8
1879	N	LEU	A	61	19.029	-33.678	31.853	1.00	31.61
1880	CA	LEU	A	61	19.332	-34.738	32.81	1.00	31.23
1881	C	LEU	A	61	18.122	-35.476	33.378	1.00	30.43
1882	O	LEU	A	61	18.26	-36.588	33.882	1.00	31.61
1883	CB	LEU	A	61	20.177	-34.171	33.957	1.00	32.54
1884	CG	LEU	A	61	21.567	-33.665	33.559	1.00	34.14
1885	CD1	LEU	A	61	22.195	-32.902	34.72	1.00	34.55
1886	CD2	LEU	A	61	22.443	-34.846	33.15	1.00	34.19
1887	N	ASN	A	62	16.939	-34.878	33.286	1.00	28.18
1888	CA	ASN	A	62	15.736	-35.508	33.827	1.00	27.26
1889	C	ASN	A	62	14.868	-36.09	32.718	1.00	26.87
1890	O	ASN	A	62	13.732	-36.489	32.953	1.00	27.3
1891	CB	ASN	A	62	14.926	-34.471	34.607	1.00	25.49
1892	CG	ASN	A	62	14.414	-33.354	33.717	1.00	25.82
1893	OD1	ASN	A	62	15.12	-32.889	32.823	1.00	25.42
1894	ND2	ASN	A	62	13.187	-32.915	33.958	1.00	25.84
1895	N	CYS	A	63	15.425	-36.161	31.518	1.00	26.73
1896	CA	CYS	A	63	14.696	-36.631	30.349	1.00	26.93
1897	C	CYS	A	63	14.941	-38.094	29.962	1.00	27.35
1898	O	CYS	A	63	16.08	-38.54	29.902	1.00	26.09
1899	CB	CYS	A	63	15.051	-35.715	29.17	1.00	26.13
1900	SG	CYS	A	63	14.132	-35.974	27.638	1.00	26.23
1901	N	ASP	A	64	13.859	-38.825	29.682	1.00	28.43
1902	CA	ASP	A	64	13.956	-40.227	29.262	1.00	28.83
1903	C	ASP	A	64	14.452	-40.27	27.819	1.00	28.7
1904	O	ASP	A	64	14.145	-39.377	27.025	1.00	27.95
1905	CB	ASP	A	64	12.589	-40.917	29.324	1.00	30.28
1906	CG	ASP	A	64	12.678	-42.422	29.07	1.00	32.76
1907	OD1	ASP	A	64	12.992	-43.165	30.029	1.00	35.08
1908	OD2	ASP	A	64	12.447	-42.862	27.916	1.00	32.26
1909	N	ASP	A	65	15.213	-41.313	27.49	1.00	28.44
1910	CA	ASP	A	65	15.752	-41.493	26.148	1.00	29.21



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1911	C	ASP	A	65	14.712	-41.353	25.033	1.00	28.8
1912	O	ASP	A	65	15.008	-40.79	23.98	1.00	28.42
1913	CB	ASP	A	65	16.413	-42.872	26.005	1.00	31.64
1914	CG	ASP	A	65	17.734	-42.973	26.737	1.00	34.16
1915	OD1	ASP	A	65	18.476	-41.973	26.76	1.00	34.59
1916	OD2	ASP	A	65	18.042	-44.059	27.271	1.00	37.13
1917	N	GLU	A	66	13.503	-41.865	25.247	1.00	26.6
1918	CA	GLU	A	66	12.49	-41.781	24.198	1.00	26.71
1919	C	GLU	A	66	12.068	-40.341	23.885	1.00	25.42
1920	O	GLU	A	66	11.869	-39.992	22.72	1.00	25.59
1921	CB	GLU	A	66	11.258	-42.614	24.558	1.00	27.86
1922	CG	GLU	A	66	10.504	-43.081	23.32	1.00	31.4
1923	CD	GLU	A	66	9.174	-43.748	23.628	1.00	32.8
1924	OE1	GLU	A	66	9.021	-44.322	24.731	1.00	32.41
1925	OE2	GLU	A	66	8.285	-43.708	22.747	1.00	33.72
1926	N	VAL	A	67	11.937	-39.507	24.914	1.00	23.68
1927	CA	VAL	A	67	11.554	-38.118	24.707	1.00	23.26
1928	C	VAL	A	67	12.655	-37.385	23.937	1.00	23.44
1929	O	VAL	A	67	12.373	-36.57	23.057	1.00	23
1930	CB	VAL	A	67	11.295	-37.384	26.052	1.00	23.27
1931	CG1	VAL	A	67	10.904	-35.942	25.788	1.00	21.07
1932	CG2	VAL	A	67	10.18	-38.083	26.834	1.00	21.69
1933	N	TYR	A	68	13.909	-37.679	24.264	1.00	23.82
1934	CA	TYR	A	68	15.033	-37.041	23.586	1.00	23.87
1935	C	TYR	A	68	15.095	-37.456	22.113	1.00	24.24
1936	O	TYR	A	68	15.362	-36.632	21.238	1.00	22.9
1937	CB	TYR	A	68	16.358	-37.399	24.277	1.00	22.46
1938	CG	TYR	A	68	17.555	-36.655	23.715	1.00	22.3
1939	CD1	TYR	A	68	17.617	-35.266	23.763	1.00	22.15
1940	CD2	TYR	A	68	18.624	-37.343	23.132	1.00	23.37
1941	CE1	TYR	A	68	18.713	-34.572	23.245	1.00	21.77
1942	CE2	TYR	A	68	19.725	-36.658	22.61	1.00	21.72
1943	CZ	TYR	A	68	19.758	-35.278	22.671	1.00	22.73
1944	OH	TYR	A	68	20.829	-34.59	22.155	1.00	23.56
1945	N	ASP	A	69	14.855	-38.733	21.836	1.00	25.77
1946	CA	ASP	A	69	14.898	-39.189	20.456	1.00	28.61
1947	C	ASP	A	69	13.809	-38.498	19.636	1.00	27.82
1948	O	ASP	A	69	13.994	-38.234	18.452	1.00	28.06
1949	CB	ASP	A	69	14.771	-40.715	20.383	1.00	32.12

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

1950	CG	ASP	A	69	16.004	-41.42	20.934	1.00	37.87
1951	OD1	ASP	A	69	17.138	-40.951	20.66	1.00	38.54
1952	OD2	ASP	A	69	15.846	-42.447	21.631	1.00	42.22
1953	N	LEU	A	70	12.68	-38.201	20.272	1.00	26.43
1954	CA	LEU	A	70	11.598	-37.496	19.597	1.00	25.47
1955	C	LEU	A	70	12.182	-36.138	19.189	1.00	25.48
1956	O	LEU	A	70	12.002	-35.68	18.059	1.00	25.42
1957	CB	LEU	A	70	10.408	-37.312	20.55	1.00	24.5
1958	CG	LEU	A	70	9.16	-36.612	19.998	1.00	24.52
1959	CD1	LEU	A	70	8.837	-37.132	18.603	1.00	23.8
1960	CD2	LEU	A	70	7.985	-36.846	20.945	1.00	22.98
1961	N	MET	A	71	12.889	-35.509	20.126	1.00	24.31
1962	CA	MET	A	71	13.544	-34.224	19.89	1.00	24.62
1963	C	MET	A	71	14.51	-34.305	18.714	1.00	24.4
1964	O	MET	A	71	14.511	-33.441	17.832	1.00	25.14
1965	CB	MET	A	71	14.349	-33.791	21.122	1.00	23.94
1966	CG	MET	A	71	13.552	-33.203	22.26	1.00	23.59
1967	SD	MET	A	71	14.652	-32.748	23.625	1.00	22.97
1968	CE	MET	A	71	13.549	-33.008	25.023	1.00	24.1
1969	N	ARG	A	72	15.346	-35.339	18.716	1.00	24.47
1970	CA	ARG	A	72	16.335	-35.522	17.658	1.00	24.74
1971	C	ARG	A	72	15.707	-35.71	16.279	1.00	24.24
1972	O	ARG	A	72	16.26	-35.255	15.276	1.00	23.61
1973	CB	ARG	A	72	17.255	-36.7	18.005	1.00	25.76
1974	CG	ARG	A	72	18.086	-36.461	19.272	1.00	27.99
1975	CD	ARG	A	72	18.986	-35.239	19.118	1.00	27.55
1976	NE	ARG	A	72	19.942	-35.429	18.032	1.00	29.65
1977	CZ	ARG	A	72	21.232	-35.703	18.209	1.00	30.61
1978	NH1	ARG	A	72	21.726	-35.811	19.432	1.00	30.4
1979	NH2	ARG	A	72	22.024	-35.887	17.162	1.00	30.6
1980	N	GLN	A	73	14.557	-36.375	16.224	1.00	23.87
1981	CA	GLN	A	73	13.866	-36.564	14.951	1.00	24.76
1982	C	GLN	A	73	13.497	-35.178	14.404	1.00	24.57
1983	O	GLN	A	73	13.633	-34.919	13.206	1.00	24.24
1984	CB	GLN	A	73	12.583	-37.382	15.133	1.00	27.21
1985	CG	GLN	A	73	12.743	-38.739	15.807	1.00	31.2
1986	CD	GLN	A	73	11.398	-39.431	16.042	1.00	34.67
1987	OE1	GLN	A	73	11.273	-40.31	16.905	1.00	36.88
1988	NE2	GLN	A	73	10.389	-39.042	15.27	1.00	34.68

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

1989	N	CYS	A	74	13.035	-34.292	15.292	1.00	23.02
1990	CA	CYS	A	74	12.643	-32.937	14.903	1.00	22.85
1991	C	CYS	A	74	13.806	-32.082	14.388	1.00	22.69
1992	O	CYS	A	74	13.574	-31.094	13.692	1.00	21.22
1993	CB	CYS	A	74	11.972	-32.193	16.071	1.00	21.64
1994	SG	CYS	A	74	10.41	-32.904	16.709	1.00	22.65
1995	N	TRP	A	75	15.047	-32.457	14.71	1.00	23.32
1996	CA	TRP	A	75	16.208	-31.674	14.268	1.00	23.64
1997	C	TRP	A	75	17.055	-32.318	13.163	1.00	25.54
1998	O	TRP	A	75	18.209	-31.93	12.951	1.00	25.5
1999	CB	TRP	A	75	17.118	-31.33	15.457	1.00	22.69
2000	CG	TRP	A	75	16.391	-30.7	16.613	1.00	24.93
2001	CD1	TRP	A	75	15.365	-29.786	16.546	1.00	23.12
2002	CD2	TRP	A	75	16.61	-30.954	18.008	1.00	24.01
2003	NE1	TRP	A	75	14.932	-29.469	17.811	1.00	24.05
2004	CE2	TRP	A	75	15.675	-30.17	18.728	1.00	24.24
2005	CE3	TRP	A	75	17.499	-31.768	18.72	1.00	24.51
2006	CZ2	TRP	A	75	15.606	-30.181	20.124	1.00	22.73
2007	CZ3	TRP	A	75	17.431	-31.778	20.114	1.00	24.02
2008	CH2	TRP	A	75	16.489	-30.988	20.798	1.00	24.4
2009	N	ARG	A	76	16.496	-33.293	12.455	1.00	27.06
2010	CA	ARG	A	76	17.243	-33.927	11.369	1.00	29.23
2011	C	ARG	A	76	17.567	-32.862	10.326	1.00	29.3
2012	O	ARG	A	76	16.776	-31.945	10.094	1.00	27.98
2013	CB	ARG	A	76	16.422	-35.067	10.761	1.00	30.76
2014	CG	ARG	A	76	16.338	-36.286	11.671	1.00	34.42
2015	CD	ARG	A	76	15.187	-37.205	11.306	1.00	38.64
2016	NE	ARG	A	76	15.136	-38.379	12.18	1.00	42.8
2017	CZ	ARG	A	76	14.083	-39.189	12.292	1.00	44.32
2018	NH1	ARG	A	76	14.132	-40.232	13.113	1.00	44.59
2019	NH2	ARG	A	76	12.978	-38.95	11.596	1.00	43.21
2020	N	GLU	A	77	18.738	-32.969	9.715	1.00	30.24
2021	CA	GLU	A	77	19.164	-31.994	8.72	1.00	32.61
2022	C	GLU	A	77	18.199	-31.927	7.531	1.00	32.6
2023	O	GLU	A	77	17.808	-30.841	7.089	1.00	30.97
2024	CB	GLU	A	77	20.583	-32.321	8.237	1.00	34.9
2025	CG	GLU	A	77	21.227	-31.214	7.429	1.00	41.76
2026	CD	GLU	A	77	22.697	-31.477	7.141	1.00	46.9
2027	OE1	GLU	A	77	23.481	-31.607	8.109	1.00	49.95

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

2028	OE2	GLU	A	77	23.074	-31.552	5.949	1.00	49.03
2029	N	LYS	A	78	17.814	-33.086	7.014	1.00	32.39
2030	CA	LYS	A	78	16.894	-33.128	5.888	1.00	33.67
2031	C	LYS	A	78	15.502	-32.783	6.391	1.00	32.38
2032	O	LYS	A	78	14.92	-33.516	7.185	1.00	32.71
2033	CB	LYS	A	78	16.914	-34.518	5.247	1.00	35.43
2034	CG	LYS	A	78	18.274	-34.864	4.644	1.00	37.54
2035	CD	LYS	A	78	18.278	-36.249	4.023	1.00	40.67
2036	CE	LYS	A	78	19.666	-36.63	3.528	1.00	41.1
2037	NZ	LYS	A	78	19.678	-38.007	2.955	1.00	43.72
2038	N	PRO	A	79	14.959	-31.643	5.948	1.00	31.94
2039	CA	PRO	A	79	13.623	-31.214	6.378	1.00	32.24
2040	C	PRO	A	79	12.558	-32.293	6.205	1.00	33.02
2041	O	PRO	A	79	11.753	-32.53	7.107	1.00	32.48
2042	CB	PRO	A	79	13.352	-29.989	5.504	1.00	30.32
2043	CG	PRO	A	79	14.725	-29.423	5.276	1.00	30.5
2044	CD	PRO	A	79	15.557	-30.665	5.019	1.00	30.71
2045	N	TYR	A	80	12.566	-32.945	5.045	1.00	33.8
2046	CA	TYR	A	80	11.596	-33.988	4.738	1.00	35.66
2047	C	TYR	A	80	11.74	-35.272	5.555	1.00	36
2048	O	TYR	A	80	10.908	-36.173	5.435	1.00	36.67
2049	CB	TYR	A	80	11.631	-34.309	3.234	1.00	37.88
2050	CG	TYR	A	80	13.02	-34.514	2.662	1.00	39.67
2051	CD1	TYR	A	80	13.659	-35.75	2.748	1.00	41.59
2052	CD2	TYR	A	80	13.693	-33.468	2.032	1.00	40.61
2053	CE1	TYR	A	80	14.939	-35.942	2.215	1.00	42.08
2054	CE2	TYR	A	80	14.967	-33.646	1.5	1.00	42.1
2055	CZ	TYR	A	80	15.583	-34.885	1.593	1.00	42.53
2056	OH	TYR	A	80	16.839	-35.062	1.055	1.00	43.97
2057	N	GLU	A	81	12.776	-35.366	6.386	1.00	34.87
2058	CA	GLU	A	81	12.944	-36.556	7.21	1.00	34.22
2059	C	GLU	A	81	12.353	-36.354	8.606	1.00	32.84
2060	O	GLU	A	81	12.178	-37.309	9.359	1.00	31.96
2061	CB	GLU	A	81	14.422	-36.943	7.321	1.00	37.26
2062	CG	GLU	A	81	15.046	-37.366	5.994	1.00	40.88
2063	CD	GLU	A	81	16.371	-38.084	6.17	1.00	43.23
2064	OE1	GLU	A	81	17.273	-37.505	6.843	1.00	44.2
2065	OE2	GLU	A	81	16.51	-39.201	5.63	1.00	44.78
2066	N	ARG	A	82	12.039	-35.109	8.947	1.00	30.55

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TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

2067	CA	ARG	A	82	11.458	-34.818	10.25	1.00	29.23
2068	C	ARG	A	82	10.032	-35.357	10.326	1.00	28.42
2069	O	ARG	A	82	9.322	-35.418	9.32	1.00	29.01
2070	CB	ARG	A	82	11.453	-33.307	10.496	1.00	28.42
2071	CG	ARG	A	82	12.839	-32.701	10.445	1.00	26.51
2072	CD	ARG	A	82	12.819	-31.196	10.4	1.00	23.95
2073	NE	ARG	A	82	14.135	-30.719	10.003	1.00	23.91
2074	CZ	ARG	A	82	14.389	-29.505	9.532	1.00	24.35
2075	NH1	ARG	A	82	13.411	-28.616	9.401	1.00	24.2
2076	NH2	ARG	A	82	15.624	-29.199	9.152	1.00	23.1
2077	N	PRO	A	83	9.593	-35.763	11.524	1.00	27.4
2078	CA	PRO	A	83	8.228	-36.279	11.635	1.00	26.93
2079	C	PRO	A	83	7.211	-35.158	11.422	1.00	27.17
2080	O	PRO	A	83	7.558	-33.973	11.457	1.00	26.32
2081	CB	PRO	A	83	8.189	-36.837	13.056	1.00	26.66
2082	CG	PRO	A	83	9.103	-35.907	13.795	1.00	26.71
2083	CD	PRO	A	83	10.267	-35.758	12.835	1.00	27
2084	N	SER	A	84	5.963	-35.535	11.178	1.00	25.83
2085	CA	SER	A	84	4.905	-34.551	10.991	1.00	25.08
2086	C	SER	A	84	4.357	-34.31	12.388	1.00	24.41
2087	O	SER	A	84	4.625	-35.089	13.299	1.00	23.97
2088	CB	SER	A	84	3.792	-35.121	10.116	1.00	25.45
2089	OG	SER	A	84	3.213	-36.249	10.752	1.00	26.24
2090	N	PHE	A	85	3.589	-33.245	12.562	1.00	23.41
2091	CA	PHE	A	85	3.019	-32.968	13.868	1.00	23.61
2092	C	PHE	A	85	2.065	-34.073	14.302	1.00	23.8
2093	O	PHE	A	85	1.921	-34.339	15.493	1.00	24.58
2094	CB	PHE	A	85	2.312	-31.611	13.866	1.00	22.93
2095	CG	PHE	A	85	3.251	-30.447	13.984	1.00	21.63
2096	CD1	PHE	A	85	3.982	-30.246	15.159	1.00	21.11
2097	CD2	PHE	A	85	3.433	-29.569	12.92	1.00	21.7
2098	CE1	PHE	A	85	4.382	-29.187	15.273	1.00	20.16
2099	CE2	PHE	A	85	4.334	-28.5	13.021	1.00	22.72
2100	CZ	PHE	A	85	5.061	-28.312	14.205	1.00	21.8
2101	N	ALA	A	86	1.422	-34.728	13.342	1.00	24.29
2102	CA	ALA	A	86	0.5	-35.821	13.668	1.00	24.78
2103	C	ALA	A	86	1.281	-37.004	14.242	1.00	24.22
2104	O	ALA	A	86	0.843	-37.64	15.203	1.00	24.91
2105	CB	ALA	A	86	-0.279	-36.262	12.413	1.00	24.72

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

2106	N	GLN	A	87	2.432	-37.304	13.649	1.00	24.02
2107	CA	GLN	A	87	3.26	-38.41	14.129	1.00	24.07
2108	C	GLN	A	87	3.781	-38.075	15.52	1.00	24.1
2109	O	GLN	A	87	3.828	-38.938	16.401	1.00	25.23
2110	CB	GLN	A	87	4.428	-38.662	13.171	1.00	25.13
2111	CG	GLN	A	87	3.99	-39.138	11.789	1.00	27.2
2112	CD	GLN	A	87	5.148	-39.291	10.82	1.00	28.59
2113	OE1	GLN	A	87	5.931	-38.365	10.624	1.00	29
2114	NE2	GLN	A	87	5.251	-40.459	10.198	1.00	29.44
2115	N	ILE	A	88	4.16	-36.814	15.717	1.00	23.01
2116	CA	ILE	A	88	4.66	-36.359	17.01	1.00	21.13
2117	C	ILE	A	88	3.586	-36.564	18.079	1.00	21.03
2118	O	ILE	A	88	3.882	-36.996	19.191	1.00	19.94
2119	CB	ILE	A	88	5.05	-34.859	16.958	1.00	20.83
2120	CG1	ILE	A	88	6.28	-34.681	16.068	1.00	19.13
2121	CG2	ILE	A	88	5.301	-34.319	18.375	1.00	18.37
2122	CD1	ILE	A	88	6.641	-33.225	15.804	1.00	19.22
2123	N	LEU	A	89	2.339	-36.258	17.734	1.00	20.47
2124	CA	LEU	A	89	1.242	-36.416	18.677	1.00	22.29
2125	C	LEU	A	89	1.021	-37.896	19.017	1.00	22.53
2126	O	LEU	A	89	0.722	-38.24	20.161	1.00	23.48
2127	CB	LEU	A	89	-0.038	-35.805	18.105	1.00	22.49
2128	CG	LEU	A	89	-1.265	-35.854	19.023	1.00	25.15
2129	CD1	LEU	A	89	-0.98	-35.115	20.332	1.00	23.77
2130	CD2	LEU	A	89	-2.453	-35.233	18.308	1.00	24.36
2131	N	VAL	A	90	1.163	-38.772	18.028	1.00	24.41
2132	CA	VAL	A	90	0.996	-40.206	18.276	1.00	24.99
2133	C	VAL	A	90	2.076	-40.669	19.252	1.00	25.11
2134	O	VAL	A	90	1.789	-41.39	20.21	1.00	23.43
2135	CB	VAL	A	90	1.097	-41.037	16.977	1.00	24.65
2136	CG1	VAL	A	90	1.3	-42.521	17.315	1.00	24.99
2137	CG2	VAL	A	90	-0.186	-40.878	16.17	1.00	24.2
2138	N	SER	A	91	3.313	-40.245	19.01	1.00	24.4
2139	CA	SER	A	91	4.412	-40.605	19.891	1.00	24.91
2140	C	SER	A	91	4.113	-40.109	21.305	1.00	25.93
2141	O	SER	A	91	4.238	-40.858	22.278	1.00	26.66
2142	CB	SER	A	91	5.721	-39.988	19.397	1.00	24.31
2143	OG	SER	A	91	6.08	-40.51	18.124	1.00	26.17
2144	N	LEU	A	92	3.696	-38.852	21.426	1.00	25.6

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

2145	CA	LEU	A	92	3.407	-38.31	22.751	1.00	25.82
2146	C	LEU	A	92	2.292	-39.064	23.477	1.00	26.2
2147	O	LEU	A	92	2.411	-39.357	24.67	1.00	24.29
2148	CB	LEU	A	92	3.064	-36.82	22.661	1.00	23.68
2149	CG	LEU	A	92	4.258	-35.918	22.328	1.00	24.58
2150	CD1	LEU	A	92	3.768	-34.506	22.051	1.00	23.64
2151	CD2	LEU	A	92	5.262	-35.942	23.477	1.00	21.58
2152	N	ASN	A	93	1.218	-39.382	22.76	1.00	26.66
2153	CA	ASN	A	93	0.101	-40.091	23.37	1.00	28.58
2154	C	ASN	A	93	0.458	-41.489	23.87	1.00	29.25
2155	O	ASN	A	93	-0.073	-41.934	24.888	1.00	29.81
2156	CB	ASN	A	93	-1.081	-40.178	22.399	1.00	29.59
2157	CG	ASN	A	93	-1.797	-38.853	22.241	1.00	29.65
2158	OD1	ASN	A	93	-1.924	-38.095	23.196	1.00	32.76
2159	ND2	ASN	A	93	-2.282	-38.575	21.041	1.00	31.59
2160	N	ARG	A	94	1.354	-42.179	23.169	1.00	29.34
2161	CA	ARG	A	94	1.747	-43.518	23.592	1.00	31.36
2162	C	ARG	A	94	2.452	-43.426	24.948	1.00	32.69
2163	O	ARG	A	94	2.189	-44.231	25.846	1.00	33.23
2164	CB	ARG	A	94	2.658	-44.169	22.541	1.00	31.07
2165	CG	ARG	A	94	2.145	-43.964	21.119	1.00	31.99
2166	CD	ARG	A	94	1.84	-45.235	20.334	1.00	31.68
2167	NE	ARG	A	94	2.982	-45.672	19.538	1.00	32.22
2168	CZ	ARG	A	94	2.907	-46.466	18.47	1.00	30.69
2169	NH1	ARG	A	94	1.739	-46.924	18.042	1.00	30.31
2170	NH2	ARG	A	94	4.011	-46.807	17.828	1.00	30.21
2171	N	MET	A	95	3.323	-42.429	25.111	1.00	32.86
2172	CA	MET	A	95	4.026	-42.259	26.38	1.00	33.26
2173	C	MET	A	95	3.061	-41.875	27.495	1.00	33.73
2174	O	MET	A	95	3.185	-42.361	28.619	1.00	33.83
2175	CB	MET	A	95	5.131	-41.207	26.26	1.00	32.83
2176	CG	MET	A	95	6.306	-41.659	25.409	1.00	34.3
2177	SD	MET	A	95	7.628	-40.428	25.253	1.00	35.36
2178	CE	MET	A	95	6.952	-39.36	24.015	1.00	33.28
2179	N	LEU	A	96	2.096	-41.014	27.187	1.00	34.36
2180	CA	LEU	A	96	1.122	-40.596	28.193	1.00	36.97
2181	C	LEU	A	96	0.259	-41.764	28.682	1.00	39.36
2182	O	LEU	A	96	-0.188	-41.779	29.831	1.00	39.76
2183	CB	LEU	A	96	0.231	-39.473	27.642	1.00	35.66

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

2184	CG	LEU	A	96	0.822	-38.053	27.667	1.00	34.59
2185	CD1	LEU	A	96	-0.057	-37.105	26.867	1.00	33.25
2186	CD2	LEU	A	96	0.948	-37.575	29.109	1.00	33.45
2187	N	GLU	A	97	0.045	-42.744	27.808	1.00	42.05
2188	CA	GLU	A	97	-0.754	-43.934	28.112	1.00	45.27
2189	C	GLU	A	97	-0.16	-44.814	29.22	1.00	45.89
2190	O	GLU	A	97	-0.889	-45.385	30.033	1.00	45.85
2191	CB	GLU	A	97	-0.914	-44.777	26.836	1.00	47.66
2192	CG	GLU	A	97	-1.095	-46.281	27.075	1.00	51.31
2193	CD	GLU	A	97	-0.418	-47.147	26.005	1.00	53.96
2194	OE1	GLU	A	97	-0.392	-48.392	26.173	1.00	54.59
2195	OE2	GLU	A	97	0.087	-46.587	25.002	1.00	53.12
2196	N	GLU	A	98	1.163	-44.919	29.247	1.00	46.18
2197	CA	GLU	A	98	1.852	-45.758	30.219	1.00	47.12
2198	C	GLU	A	98	2.073	-45.116	31.595	1.00	47.52
2199	O	GLU	A	98	2.1	-43.892	31.733	1.00	47.65
2200	CB	GLU	A	98	3.18	-46.212	29.605	1.00	47.71
2201	CG	GLU	A	98	3.008	-46.671	28.155	1.00	49.28
2202	CD	GLU	A	98	4.314	-46.992	27.455	1.00	50.3
2203	OE1	GLU	A	98	5.302	-46.263	27.667	1.00	51.38
2204	OE2	GLU	A	98	4.348	-47.965	26.673	1.00	50.93
2205	N	ALA	A	99	2.225	-45.96	32.612	1.00	47.72
2206	CA	ALA	A	99	2.433	-45.499	33.984	1.00	47.92
2207	C	ALA	A	99	3.84	-44.945	34.197	1.00	47.61
2208	O	ALA	A	99	4.08	-44.165	35.121	1.00	48.92
2209	CB	ALA	A	99	2.169	-46.648	34.963	1.00	47.81
2210	N	LYS	A	100	4.763	-45.353	33.335	1.00	45.75
2211	CA	LYS	A	100	6.154	-44.918	33.399	1.00	43.91
2212	C	LYS	A	100	6.311	-43.39	33.351	1.00	42.21
2213	O	LYS	A	100	5.565	-42.698	32.657	1.00	41.79
2214	CB	LYS	A	100	6.929	-45.564	32.243	1.00	44.02
2215	CG	LYS	A	100	8.405	-45.226	32.183	1.00	45.18
2216	CD	LYS	A	100	9.087	-45.937	31.019	1.00	45.26
2217	CE	LYS	A	100	10.568	-45.596	30.96	1.00	46.19
2218	NZ	LYS	A	100	11.265	-46.311	29.855	1.00	47.56
2219	N	THR	A	101	7.282	-42.88	34.107	1.00	40.07
2220	CA	THR	A	101	7.593	-41.45	34.165	1.00	37.76
2221	C	THR	A	101	8.606	-41.133	33.067	1.00	36.91
2222	O	THR	A	101	9.683	-41.736	33.025	1.00	37.75



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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

2223	CB	THR	A	101	8.226	-41.076	35.524	1.00	37.83
2224	OG1	THR	A	101	7.237	-41.161	36.554	1.00	37.73
2225	CG2	THR	A	101	8.811	-39.667	35.484	1.00	37.83
2226	N	TYR	A	102	8.279	-40.19	32.185	1.00	34.63
2227	CA	TYR	A	102	9.192	-39.846	31.096	1.00	31.89
2228	C	TYR	A	102	10.005	-38.584	31.323	1.00	30.02
2229	O	TYR	A	102	11.129	-38.467	30.837	1.00	29.4
2230	CB	TYR	A	102	8.427	-39.748	29.769	1.00	31.82
2231	CG	TYR	A	102	8.115	-41.105	29.186	1.00	32.53
2232	CD1	TYR	A	102	6.934	-41.777	29.517	1.00	32.71
2233	CD2	TYR	A	102	9.044	-41.764	28.379	1.00	32.71
2234	CE1	TYR	A	102	6.688	-43.072	29.065	1.00	32.25
2235	CE2	TYR	A	102	8.812	-43.059	27.925	1.00	33.33
2236	CZ	TYR	A	102	7.633	-43.707	28.274	1.00	33.59
2237	OH	TYR	A	102	7.412	-44.995	27.852	1.00	33.69
2238	N	VAL	A	103	9.431	-37.639	32.052	1.00	28.58
2239	CA	VAL	A	103	10.108	-36.391	32.358	1.00	28.14
2240	C	VAL	A	103	10.152	-36.316	33.87	1.00	28.3
2241	O	VAL	A	103	9.158	-35.961	34.504	1.00	29.78
2242	CB	VAL	A	103	9.327	-35.179	31.827	1.00	28.54
2243	CG1	VAL	A	103	10.093	-33.906	32.125	1.00	27.92
2244	CG2	VAL	A	103	9.084	-35.326	30.331	1.00	27.84
2245	N	ASN	A	104	11.298	-36.647	34.45	1.00	26.47
2246	CA	ASN	A	104	11.416	-36.642	35.899	1.00	27.43
2247	C	ASN	A	104	11.392	-35.292	36.593	1.00	27.53
2248	O	ASN	A	104	12.009	-34.325	36.135	1.00	25.68
2249	CB	ASN	A	104	12.679	-37.37	36.343	1.00	27.46
2250	CG	ASN	A	104	12.818	-37.391	37.851	1.00	29.12
2251	OD1	ASN	A	104	11.954	-37.917	38.55	1.00	30.02
2252	ND2	ASN	A	104	13.895	-36.807	38.362	1.00	26.71
2253	N	THR	A	105	10.671	-35.246	37.709	1.00	28.18
2254	CA	THR	A	105	10.571	-34.046	38.528	1.00	29.17
2255	C	THR	A	105	10.759	-34.426	39.995	1.00	29.05
2256	O	THR	A	105	10.586	-33.595	40.882	1.00	29.14
2257	CB	THR	A	105	9.206	-33.332	38.37	1.00	29.06
2258	OG1	THR	A	105	8.149	-34.22	38.751	1.00	30.8
2259	CG2	THR	A	105	9.009	-32.871	36.93	1.00	29.37
2260	N	THR	A	106	11.105	-35.688	40.24	1.00	30.06
2261	CA	THR	A	106	11.338	-36.184	41.598	1.00	30.21

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

2262	C	THR	A	106	12.801	-35.976	41.962	1.00	30.32
2263	O	THR	A	106	13.698	-36.326	41.192	1.00	29.1
2264	CB	THR	A	106	11.001	-37.682	41.714	1.00	30.19
2265	CG1	THR	A	106	9.602	-37.868	41.484	1.00	30.25
2266	CG2	THR	A	106	11.346	-38.204	43.1	1.00	30.15
2267	N	LEU	A	107	13.039	-35.415	43.142	1.00	31.35
2268	CA	LEU	A	107	14.401	-35.13	43.583	1.00	33.51
2269	C	LEU	A	107	15.348	-36.328	43.68	1.00	34.81
2270	O	LEU	A	107	16.441	-36.302	43.105	1.00	35.34
2271	CB	LEU	A	107	14.373	-34.393	44.925	1.00	32.24
2272	CG	LEU	A	107	13.686	-33.023	44.912	1.00	32.89
2273	CD1	LEU	A	107	13.753	-32.418	46.299	1.00	32.92
2274	CD2	LEU	A	107	14.361	-32.103	43.897	1.00	31.51
2275	N	TYR	A	108	14.933	-37.372	44.397	1.00	35.78
2276	CA	TYR	A	108	15.777	-38.549	44.595	1.00	37.04
2277	C	TYR	A	108	17.061	-38.086	45.28	1.00	38.1
2278	O	TYR	A	108	17.001	-37.459	46.337	1.00	38.13
2279	CB	TYR	A	108	16.089	-39.238	43.26	1.00	37.75
2280	CG	TYR	A	108	14.879	-39.894	42.622	1.00	39.28
2281	CD1	TYR	A	108	14.571	-39.678	41.28	1.00	39.26
2282	CD2	TYR	A	108	14.027	-40.711	43.37	1.00	40.73
2283	CE1	TYR	A	108	13.446	-40.25	40.697	1.00	39.71
2284	CE2	TYR	A	108	12.895	-41.293	42.795	1.00	41.43
2285	CZ	TYR	A	108	12.612	-41.054	41.457	1.00	41.06
2286	OH	TYR	A	108	11.487	-41.598	40.883	1.00	40.87
2287	N	GLU	A	109	18.217	-38.363	44.687	1.00	39.28
2288	CA	GLU	A	109	19.467	-37.95	45.312	1.00	41.05
2289	C	GLU	A	109	20.201	-36.805	44.628	1.00	40.2
2290	O	GLU	A	109	21.228	-36.336	45.124	1.00	39.49
2291	CB	GLU	A	109	20.4	-39.155	45.471	1.00	44.38
2292	CG	GLU	A	109	20.003	-40.05	46.647	1.00	49.94
2293	CD	GLU	A	109	21.111	-40.991	47.087	1.00	53.49
2294	OE1	GLU	A	109	21.025	-41.511	48.225	1.00	54.77
2295	OE2	GLU	A	109	22.08	-41.215	46.298	1.00	55.3
2296	N	LYS	A	110	19.671	-36.343	43.502	1.00	38.82
2297	CA	LYS	A	110	20.301	-35.248	42.781	1.00	37.84
2298	C	LYS	A	110	19.42	-34.725	41.652	1.00	36.67
2299	O	LYS	A	110	18.866	-35.505	40.875	1.00	36.14
2300	CB	LYS	A	110	21.646	-35.707	42.209	1.00	39.93

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

2301	CG	LYS	A	110	22.448	-34.608	41.533	1.00	42.26
2302	CD	LYS	A	110	23.769	-35.141	41.005	1.00	45.3
2303	CE	LYS	A	110	24.613	-34.024	40.402	1.00	47.5
2304	NZ	LYS	A	110	25.899	-34.534	39.833	1.00	49.55
2305	N	PHE	A	111	19.287	-33.404	41.572	1.00	34.71
2306	CA	PHE	A	111	18.497	-32.785	40.517	1.00	33.05
2307	C	PHE	A	111	19.102	-31.442	40.127	1.00	32.55
2308	O	PHE	A	111	19.456	-30.628	40.985	1.00	31.01
2309	CB	PHE	A	111	17.043	-32.603	40.951	1.00	32.12
2310	CG	PHE	A	111	16.115	-32.273	39.81	1.00	33.04
2311	CD1	PHE	A	111	16.093	-30.995	39.255	1.00	32.77
2312	CD2	PHE	A	111	15.279	-33.251	39.272	1.00	33.12
2313	CE1	PHE	A	111	15.251	-30.694	38.182	1.00	33.2
2314	CE2	PHE	A	111	14.435	-32.961	38.199	1.00	33.13
2315	CZ	PHE	A	111	14.421	-31.678	37.653	1.00	33.17
2316	N	THR	A	112	19.214	-31.216	38.824	1.00	31.59
2317	CA	THR	A	112	19.802	-29.988	38.317	1.00	31.54
2318	C	THR	A	112	18.847	-29.18	37.444	1.00	30.61
2319	O	THR	A	112	18.219	-29.716	36.533	1.00	31.06
2320	CB	THR	A	112	21.056	-30.3	37.486	1.00	32.12
2321	OG1	THR	A	112	21.892	-31.217	38.203	1.00	32.53
2322	CG2	THR	A	112	21.828	-29.029	37.196	1.00	31.81
2323	N	TYR	A	113	18.738	-27.888	37.733	1.00	29.26
2324	CA	TYR	A	113	17.893	-26.997	36.947	1.00	27.83
2325	C	TYR	A	113	18.72	-26.492	35.775	1.00	27.96
2326	O	TYR	A	113	19.878	-26.105	35.945	1.00	27.74
2327	CB	TYR	A	113	17.439	-25.797	37.785	1.00	26.75
2328	CG	TYR	A	113	16.219	-26.039	38.64	1.00	25.09
2329	CD1	TYR	A	113	15.98	-25.258	39.765	1.00	25.51
2330	CD2	TYR	A	113	15.297	-27.04	38.324	1.00	23.93
2331	CE1	TYR	A	113	14.86	-25.464	40.563	1.00	25.42
2332	CE2	TYR	A	113	14.165	-27.254	39.114	1.00	24.19
2333	CZ	TYR	A	113	13.957	-26.463	40.234	1.00	25.27
2334	OH	TYR	A	113	12.87	-26.677	41.047	1.00	26.55
2335	N	ALA	A	114	18.129	-26.502	34.586	1.00	27.64
2336	CA	ALA	A	114	18.819	-26.024	33.393	1.00	27.07
2337	C	ALA	A	114	19.038	-24.524	33.531	1.00	26.53
2338	O	ALA	A	114	18.188	-23.81	34.065	1.00	25.9
2339	CB	ALA	A	114	17.985	-26.315	32.148	1.00	26.34

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

2340	N	GLY	A	115	20.176	-24.047	33.045	1.00	27.32
2341	CA	GLY	A	115	20.473	-22.633	33.14	1.00	29.22
2342	C	GLY	A	115	19.524	-21.727	32.374	1.00	31.97
2343	O	GLY	A	115	18.904	-22.12	31.376	1.00	30.02
2344	N	ILE	A	116	19.408	-20.502	32.867	1.00	33.91
2345	CA	ILE	A	116	18.566	-19.48	32.262	1.00	37.28
2346	C	ILE	A	116	19.473	-18.272	32.049	1.00	41.6
2347	O	ILE	A	116	19.833	-17.577	33	1.00	41.82
2348	CB	ILE	A	116	17.399	-19.097	33.197	1.00	35.59
2349	CG1	ILE	A	116	16.418	-20.264	33.304	1.00	33.13
2350	CG2	ILE	A	116	16.701	-17.843	32.686	1.00	34.99
2351	CD1	ILE	A	116	15.315	-20.046	34.316	1.00	31.79
2352	N	ASP	A	117	19.866	-18.041	30.801	1.00	46.56
2353	CA	ASP	A	117	20.747	-16.922	30.481	1.00	51.72
2354	C	ASP	A	117	19.942	-15.708	30.034	1.00	54.83
2355	O	ASP	A	117	19.742	-15.493	28.835	1.00	54.67
2356	CB	ASP	A	117	21.732	-17.325	29.38	1.00	53.37
2357	CG	ASP	A	117	22.775	-16.255	29.109	1.00	55.1
2358	OD1	ASP	A	117	23.553	-15.934	30.034	1.00	55.86
2359	OD2	ASP	A	117	22.818	-15.737	27.971	1.00	56.37
2360	N	CYS	A	118	19.479	-14.919	31.002	1.00	57.99
2361	CA	CYS	A	118	18.694	-13.725	30.707	1.00	61.55
2362	C	CYS	A	118	19.485	-12.726	29.861	1.00	62.71
2363	O	CYS	A	118	18.931	-11.739	29.369	1.00	62.7
2364	CB	CYS	A	118	18.229	-13.059	32.008	1.00	63.09
2365	SG	CYS	A	118	17.011	-14.026	32.95	1.00	66.36
2366	N	ALA	A	119	20.78	-12.991	29.697	1.00	64.01
2367	CA	ALA	A	119	21.654	-12.138	28.898	1.00	65.12
2368	C	ALA	A	119	21.533	-12.548	27.431	1.00	65.92
2369	O	ALA	A	119	22.35	-12.167	26.591	1.00	66.53
2370	CB	ALA	A	119	23.099	-12.279	29.368	1.00	64.81
2371	N	ALA	A	120	20.506	-13.341	27.142	1.00	66.3
2372	CA	ALA	A	120	20.229	-13.821	25.793	1.00	66.5
2373	C	ALA	A	120	18.716	-13.776	25.6	1.00	66.67
2374	O	ALA	A	120	18.168	-14.397	24.687	1.00	67.11
2375	CB	ALA	A	120	20.744	-15.248	25.624	1.00	65.86
2376	N	GLU	A	121	18.054	-13.033	26.481	1.00	66.47
2377	CA	GLU	A	121	16.606	-12.879	26.451	1.00	66.22
2378	C	GLU	A	121	16.22	-11.413	26.62	1.00	66.82

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

2379	O	GLU	A	121	15.698	-11.062	27.7	1.00	67.42
2380	CB	GLU	A	121	15.968	-13.72	27.561	1.00	64.72
2381	CG	GLU	A	121	15.992	-15.216	27.291	1.00	62.93
2382	CD	GLU	A	121	15.501	-16.035	28.47	1.00	61.13
2383	OE1	GLU	A	121	14.476	-15.66	29.074	1.00	59.53
2384	OE2	GLU	A	121	16.138	-17.059	28.784	1.00	60.4
2385	OXT	GLU	A	121	16.456	-10.63	25.674	1.00	67.37
2386	N	ALA	B	813	11.974	9.531	43.819	1.00	63.69
2387	CA	ALA	B	813	11.436	9.062	42.509	1.00	63.47
2388	C	ALA	B	813	9.957	8.695	42.635	1.00	63.52
2389	O	ALA	B	813	9.511	7.695	42.072	1.00	63.82
2390	CB	ALA	B	813	12.24	7.857	42.023	1.00	63.32
2391	N	THR	B	814	9.203	9.507	43.373	1.00	63.02
2392	CA	THR	B	814	7.776	9.257	43.565	1.00	62.29
2393	C	THR	B	814	6.935	10.446	43.114	1.00	62.17
2394	O	THR	B	814	7.274	11.6	43.381	1.00	61.62
2395	CB	THR	B	814	7.434	8.971	45.043	1.00	61.74
2396	OG1	THR	B	814	8.205	7.859	45.512	1.00	61.48
2397	CG2	THR	B	814	5.957	8.641	45.188	1.00	61.16
2398	N	ILE	B	815	5.836	10.155	42.424	1.00	61.87
2399	CA	ILE	B	815	4.936	11.198	41.95	1.00	61.33
2400	C	ILE	B	815	3.625	11.098	42.716	1.00	60.73
2401	O	ILE	B	815	2.995	10.04	42.761	1.00	60.91
2402	CB	ILE	B	815	4.668	11.065	40.44	1.00	61.35
2403	CG1	ILE	B	815	5.993	11.177	39.679	1.00	61.68
2404	CG2	ILE	B	815	3.696	12.154	39.983	1.00	61.76
2405	CD1	ILE	B	815	5.87	10.994	38.189	1.00	62.18
2406	N	TYR	B	816	3.22	12.208	43.321	1.00	60.05
2407	CA	TYR	B	816	1.991	12.234	44.102	1.00	59.17
2408	C	TYR	B	816	0.904	13.04	43.406	1.00	57.23
2409	O	TYR	B	816	1.19	13.851	42.52	1.00	57.01
2410	CB	TYR	B	816	2.266	12.827	45.492	1.00	61.07
2411	CG	TYR	B	816	3.51	12.279	46.159	1.00	62.77
2412	CD1	TYR	B	816	4.781	12.67	45.731	1.00	63.55
2413	CD2	TYR	B	816	3.419	11.361	47.208	1.00	63.31
2414	CE1	TYR	B	816	5.93	12.162	46.333	1.00	64.11
2415	CE2	TYR	B	816	4.564	10.845	47.816	1.00	63.99
2416	CZ	TYR	B	816	5.813	11.252	47.374	1.00	64.47
2417	OH	TYR	B	816	6.946	10.751	47.973	1.00	64.98

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

2418	N	PRO	B	817	-0.361	12.816	43.792	1.00	55.4
2419	CA	PRO	B	817	-0.726	11.85	44.835	1.00	53.94
2420	C	PRO	B	817	-0.592	10.396	44.379	1.00	52.98
2421	O	PRO	B	817	-0.59	10.099	43.182	1.00	52.31
2422	CB	PRO	B	817	-2.171	12.223	45.153	1.00	54.54
2423	CG	PRO	B	817	-2.687	12.678	43.802	1.00	54.6
2424	CD	PRO	B	817	-1.548	13.545	43.308	1.00	54.65
2425	N	VAL	B	818	-0.466	9.492	45.343	1.00	51.66
2426	CA	VAL	B	818	-0.368	8.075	45.034	1.00	49.39
2427	C	VAL	B	818	-1.797	7.63	44.743	1.00	48.27
2428	O	VAL	B	818	-2.684	7.773	45.582	1.00	48.56
2429	CB	VAL	B	818	0.186	7.274	46.228	1.00	49.56
2430	CG1	VAL	B	818	0.231	5.794	45.886	1.00	49.61
2431	CG2	VAL	B	818	1.572	7.778	46.583	1.00	49.15
2432	N	LEU	B	819	-2.019	7.102	43.548	1.00	46.41
2433	CA	LEU	B	819	-3.346	6.668	43.161	1.00	45.52
2434	C	LEU	B	819	-3.563	5.185	43.458	1.00	45.59
2435	O	LEU	B	819	-2.622	4.389	43.431	1.00	44.86
2436	CB	LEU	B	819	-3.563	6.943	41.073	1.00	44.74
2437	CG	LEU	B	819	-3.277	8.371	41.192	1.00	44.4
2438	CD1	LEU	B	819	-3.425	8.449	39.677	1.00	43.59
2439	CD2	LEU	B	819	-4.229	9.339	41.873	1.00	44.04
2440	N	ASP	B	820	-4.807	4.818	43.751	1.00	45.53
2441	CA	ASP	B	820	-5.139	3.427	44.038	1.00	45.97
2442	C	ASP	B	820	-5.611	2.747	42.765	1.00	44.29
2443	O	ASP	B	820	-6.595	3.164	42.153	1.00	44.18
2444	CB	ASP	B	820	-6.226	3.342	45.11	1.00	48.27
2445	CG	ASP	B	820	-5.711	3.705	46.487	1.00	51.42
2446	OD1	ASP	B	820	-4.757	3.046	46.962	1.00	52.67
2447	OD2	ASP	B	820	-6.258	4.644	47.109	1.00	53.98
2448	N	TRP	B	821	-4.901	1.697	42.371	1.00	42.79
2449	CA	TRP	B	821	-5.237	0.949	41.17	1.00	40.73
2450	C	TRP	B	821	-6.733	0.712	41.032	1.00	40.34
2451	O	TRP	B	821	-7.277	0.784	39.935	1.00	39.67
2452	CB	TRP	B	821	-4.498	-0.389	41.165	1.00	40.47
2453	CG	TRP	B	821	-4.91	-1.284	40.04	1.00	39.06
2454	CD1	TRP	B	821	-5.815	-2.303	40.09	1.00	38.59
2455	CD2	TRP	B	821	-4.464	-1.206	38.682	1.00	37.65
2456	NE1	TRP	B	821	-5.959	-2.871	38.846	1.00	38.91

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

2457	CE2	TRP	B	821	-5.138	-2.218	37.964	1.00	37.86
2458	CE3	TRP	B	821	-3.553	-0.385	38.004	1.00	37.39
2459	CZ2	TRP	B	821	-4.939	-2.426	36.596	1.00	37.02
2460	CZ3	TRP	B	821	-3.354	-0.591	36.642	1.00	36.87
2461	CH2	TRP	B	821	-4.043	-1.61	35.955	1.00	36.75
2462	N	ASN	B	822	-7.401	0.442	42.147	1.00	40.38
2463	CA	ASN	B	822	-8.834	0.185	42.108	1.00	40.77
2464	C	ASN	B	822	-9.664	1.396	41.705	1.00	40.15
2465	O	ASN	B	822	-10.799	1.252	41.257	1.00	40.16
2466	CB	ASN	B	822	-9.312	-0.343	43.464	1.00	42.75
2467	CG	ASN	B	822	-8.877	-1.773	43.71	1.00	44.7
2468	OD1	ASN	B	822	-9.218	-2.674	42.941	1.00	44.8
2469	ND2	ASN	B	822	-8.112	-1.989	44.781	1.00	44.96
2470	N	ASP	B	823	-9.103	2.59	41.852	1.00	39.59
2471	CA	ASP	B	823	-9.832	3.796	41.486	1.00	39.4
2472	C	ASP	B	823	-9.635	4.189	40.029	1.00	38.96
2473	O	ASP	B	823	-10.118	5.23	39.6	1.00	38.86
2474	CB	ASP	B	823	-9.418	4.964	42.379	1.00	40.06
2475	CG	ASP	B	823	-9.92	4.818	43.799	1.00	40.66
2476	OD1	ASP	B	823	-11.107	4.47	43.972	1.00	40.04
2477	OD2	ASP	B	823	-9.134	5.062	44.738	1.00	40.85
2478	N	ILE	B	824	-8.929	3.361	39.269	1.00	38.07
2479	CA	ILE	B	824	-8.675	3.664	37.868	1.00	37.25
2480	C	ILE	B	824	-9.556	2.87	36.917	1.00	37.37
2481	O	ILE	B	824	-9.641	1.651	37.003	1.00	38.58
2482	CB	ILE	B	824	-7.207	3.406	37.513	1.00	35.88
2483	CG1	ILE	B	824	-6.309	4.258	38.403	1.00	34.91
2484	CG2	ILE	B	824	-6.965	3.721	36.045	1.00	36.38
2485	CD1	ILE	B	824	-4.837	3.965	38.24	1.00	35.33
2486	N	LYS	B	825	-10.214	3.577	36.01	1.00	38.61
2487	CA	LYS	B	825	-11.087	2.952	35.029	1.00	40.13
2488	C	LYS	B	825	-10.583	3.311	33.631	1.00	39.57
2489	O	LYS	B	825	-10.55	4.486	33.261	1.00	39.84
2490	CB	LYS	B	825	-12.52	3.453	35.222	1.00	43.5
2491	CG	LYS	B	825	-13.559	2.79	34.327	1.00	48.65
2492	CD	LYS	B	825	-14.966	3.273	34.687	1.00	52.5
2493	CE	LYS	B	825	-16.049	2.573	33.864	1.00	54.09
2494	NZ	LYS	B	825	-17.424	3.07	34.2	1.00	53.59
2495	N	PHE	B	826	-10.172	2.303	32.866	1.00	38.24

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

2496	CA	PHE	B	826	-9.68	2.527	31.51	1.00	37.64
2497	C	PHE	B	826	-10.867	2.549	30.554	1.00	37.74
2498	O	PHE	B	826	-11.773	1.731	30.673	1.00	38.16
2499	CB	PHE	B	826	-8.711	1.416	31.109	1.00	36.71
2500	CG	PHE	B	826	-7.552	1.254	32.051	1.00	36.62
2501	CD1	PHE	B	826	-7.504	0.185	32.937	1.00	35.73
2502	CD2	PHE	B	826	-6.506	2.175	32.054	1.00	36.52
2503	CE1	PHE	B	826	-6.43	0.034	33.811	1.00	36.47
2504	CE2	PHE	B	826	-5.427	2.035	32.923	1.00	35.53
2505	CZ	PHE	B	826	-5.389	0.963	33.803	1.00	36.78
2506	N	GLN	B	827	-10.862	3.474	29.6	1.00	37.84
2507	CA	GLN	B	827	-11.977	3.575	28.666	1.00	38.5
2508	C	GLN	B	827	-11.616	3.47	27.188	1.00	37.6
2509	O	GLN	B	827	-12.441	3.048	26.386	1.00	37.61
2510	CB	GLN	B	827	-12.717	4.896	28.873	1.00	39.4
2511	CG	GLN	B	827	-12.939	5.283	30.318	1.00	42.6
2512	CD	GLN	B	827	-13.492	6.687	30.441	1.00	45.47
2513	OE1	GLN	B	827	-14.682	6.918	30.229	1.00	47.4
2514	NE2	GLN	B	827	-12.623	7.641	30.764	1.00	46.39
2515	N	ASP	B	828	-10.394	3.847	26.822	1.00	36.67
2516	CA	ASP	B	828	-10.005	3.826	25.417	1.00	35.31
2517	C	ASP	B	828	-8.494	3.998	25.287	1.00	34.88
2518	O	ASP	B	828	-7.795	4.232	26.27	1.00	34.53
2519	CB	ASP	B	828	-10.732	4.977	24.702	1.00	36.82
2520	CG	ASP	B	828	-10.787	4.816	23.187	1.00	37.32
2521	OD1	ASP	B	828	-11.472	5.649	22.554	1.00	38.87
2522	OD2	ASP	B	828	-10.167	3.888	22.627	1.00	36.94
2523	N	VAL	B	829	-7.996	3.875	24.063	1.00	34.32
2524	CA	VAL	B	829	-6.575	4.031	23.794	1.00	33.19
2525	C	VAL	B	829	-6.427	5.173	22.789	1.00	32.43
2526	O	VAL	B	829	-7.049	5.159	21.731	1.00	31.9
2527	CB	VAL	B	829	-5.984	2.744	23.193	1.00	33.31
2528	CG1	VAL	B	829	-4.487	2.9	22.987	1.00	32.86
2529	CG2	VAL	B	829	-6.284	1.567	24.104	1.00	34.35
2530	N	ILE	B	830	-5.606	6.161	23.126	1.00	31.19
2531	CA	ILE	B	830	-5.403	7.307	22.248	1.00	31.51
2532	C	ILE	B	830	-3.947	7.744	22.234	1.00	31.16
2533	O	ILE	B	830	-3.09	7.092	22.828	1.00	32.37
2534	CB	ILE	B	830	-6.246	8.509	22.708	1.00	31.72



TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

2535	CG1	ILE	B	830	-5.823	8.914	24.126	1.00	32.37
2536	CG2	ILE	B	830	-7.738	8.16	22.653	1.00	31.98
2537	CD1	ILE	B	830	-6.549	10.144	24.674	1.00	31.95
2538	N	GLY	B	831	-3.68	8.849	21.542	1.00	30.05
2539	CA	GLY	B	831	-2.335	9.386	21.476	1.00	27.6
2540	C	GLY	B	831	-2.323	10.721	22.197	1.00	26.99
2541	O	GLY	B	831	-3.372	11.326	22.388	1.00	25.92
2542	N	GLU	B	832	-1.151	11.177	22.615	1.00	25.47
2543	CA	GLU	B	832	-1.056	12.456	23.296	1.00	24.29
2544	C	GLU	B	832	0.345	13.049	23.155	1.00	23.58
2545	O	GLU	B	832	1.154	12.987	24.07	1.00	23.42
2546	CB	GLU	B	832	-1.444	12.297	24.778	1.00	25.07
2547	CG	GLU	B	832	-1.485	13.608	25.551	1.00	25.38
2548	CD	GLU	B	832	-2.338	13.539	26.811	1.00	27.32
2549	OE1	GLU	B	832	-2.275	14.493	27.614	1.00	27.7
2550	OE2	GLU	B	832	-3.079	12.549	27.002	1.00	26.82
2551	N	GLY	B	833	0.627	13.611	21.983	1.00	23.64
2552	CA	GLY	B	833	1.924	14.221	21.748	1.00	23
2553	C	GLY	B	833	3.083	13.278	22.003	1.00	23.6
2554	O	GLY	B	833	3.012	12.099	21.65	1.00	22.48
2555	N	ASN	B	834	4.144	13.776	22.637	1.00	22.16
2556	CA	ASN	B	834	5.294	12.923	22.884	1.00	22.53
2557	C	ASN	B	834	5.096	11.84	23.951	1.00	23.12
2558	O	ASN	B	834	6.011	11.069	24.218	1.00	23.03
2559	CB	ASN	B	834	6.548	13.764	23.161	1.00	21.6
2560	CG	ASN	B	834	6.352	14.804	24.254	1.00	21.97
2561	OD1	ASN	B	834	7.118	15.763	24.34	1.00	23.8
2562	ND2	ASN	B	834	5.343	14.617	25.095	1.00	18.94
2563	N	PHE	B	835	3.91	11.777	24.556	1.00	23.92
2564	CA	PHE	B	835	3.623	10.711	25.52	1.00	25.05
2565	C	PHE	B	835	3.327	9.439	24.714	1.00	25.36
2566	O	PHE	B	835	3.229	8.338	25.263	1.00	26.26
2567	CB	PHE	B	835	2.389	11.028	26.375	1.00	25.09
2568	CG	PHE	B	835	2.659	11.954	27.532	1.00	26.81
2569	CD1	PHE	B	835	2.418	13.323	27.423	1.00	26.7
2570	CD2	PHE	B	835	3.14	11.451	28.739	1.00	26.63
2571	CE1	PHE	B	835	2.649	14.178	28.5	1.00	27.74
2572	CE2	PHE	B	835	3.376	12.295	29.823	1.00	27.75
2573	CZ	PHE	B	835	3.129	13.662	29.704	1.00	28.55

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

2574	N	GLY	B	836	3.177	9.604	23.404	1.00	26.33
2575	CA	GLY	B	836	2.878	8.471	22.547	1.00	26.28
2576	C	GLY	B	836	1.487	7.953	22.863	1.00	26.57
2577	O	GLY	B	836	0.602	8.724	23.232	1.00	25.49
2578	N	GLN	B	837	1.291	6.647	22.728	1.00	27.23
2579	CA	GLN	B	837	-0.003	6.045	23.011	1.00	28.53
2580	C	GLN	B	837	-0.249	5.987	24.51	1.00	27.12
2581	O	GLN	B	837	0.615	5.559	25.267	1.00	27.63
2582	CB	GLN	B	837	-0.066	4.632	22.426	1.00	32.25
2583	CG	GLN	B	837	0.056	4.591	20.904	1.00	37.92
2584	CD	GLN	B	837	-1.071	5.344	20.213	1.00	40.36
2585	OE1	GLN	B	837	-2.242	4.973	20.326	1.00	42.75
2586	NE2	GLN	B	837	-0.723	6.412	19.5	1.00	41.92
2587	N	VAL	B	838	-1.423	6.438	24.934	1.00	25.03
2588	CA	VAL	B	838	-1.783	6.409	26.341	1.00	24.29
2589	C	VAL	B	838	-3.2	5.868	26.496	1.00	25.47
2590	O	VAL	B	838	-3.955	5.757	25.525	1.00	24
2591	CB	VAL	B	838	-1.715	7.817	26.99	1.00	24.12
2592	CG1	VAL	B	838	-0.281	8.343	26.959	1.00	22.65
2593	CG2	VAL	B	838	-2.653	8.776	26.267	1.00	24.11
2594	N	LEU	B	839	-3.558	5.526	27.723	1.00	26.86
2595	CA	LEU	B	839	-4.89	5.007	27.997	1.00	28.41
2596	C	LEU	B	839	-5.786	6.143	28.464	1.00	28.99
2597	O	LEU	B	839	-5.421	6.895	29.364	1.00	27.95
2598	CB	LEU	B	839	-4.814	3.934	29.083	1.00	28.7
2599	CG	LEU	B	839	-4.074	2.651	28.702	1.00	27.77
2600	CD1	LEU	B	839	-3.552	1.967	29.94	1.00	28.71
2601	CD2	LEU	B	839	-5.012	1.742	27.936	1.00	29.22
2602	N	LYS	B	840	-6.937	6.298	27.824	1.00	30.83
2603	CA	LYS	B	840	-7.873	7.329	28.239	1.00	33.04
2604	C	LYS	B	840	-8.548	6.703	29.444	1.00	34.1
2605	O	LYS	B	840	-8.928	5.529	29.395	1.00	34.41
2606	CB	LYS	B	840	-8.908	7.604	27.151	1.00	34.14
2607	CG	LYS	B	840	-9.961	8.621	27.566	1.00	36.51
2608	CD	LYS	B	840	-10.909	8.942	26.427	1.00	39.29
2609	CE	LYS	B	840	-11.987	9.932	26.868	1.00	41.62
2610	NZ	LYS	B	840	-12.837	9.377	27.96	1.00	42.21
2611	N	ALA	B	841	-8.702	7.465	30.52	1.00	34.31
2612	CA	ALA	B	841	-9.312	6.904	31.717	1.00	35.59

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

2613	C	ALA	B	841	-9.947	7.902	32.666	1.00	36.07
2614	O	ALA	B	841	-9.99	9.106	32.41	1.00	35.83
2615	CB	ALA	B	841	-8.271	6.097	32.471	1.00	35.46
2616	N	ARG	B	842	-10.452	7.359	33.767	1.00	37.12
2617	CA	ARG	B	842	-11.063	8.134	34.834	1.00	38.8
2618	C	ARG	B	842	-10.331	7.721	36.105	1.00	38.77
2619	O	ARG	B	842	-10.136	6.533	36.349	1.00	38.47
2620	CB	ARG	B	842	-12.551	7.806	34.974	1.00	39.64
2621	CG	ARG	B	842	-13.408	8.21	33.794	1.00	42.46
2622	CD	ARG	B	842	-14.691	8.872	34.277	1.00	44.97
2623	NE	ARG	B	842	-14.457	10.251	34.698	1.00	48.77
2624	CZ	ARG	B	842	-15.319	10.988	35.395	1.00	50.42
2625	NH1	ARG	B	842	-16.489	10.482	35.765	1.00	51.24
2626	NH2	ARG	B	842	-15.015	12.239	35.714	1.00	51.72
2627	N	ILE	B	843	-9.906	8.696	36.899	1.00	40.06
2628	CA	ILE	B	843	-9.2	8.413	38.144	1.00	41.33
2629	C	ILE	B	843	-9.924	9.094	39.297	1.00	43.26
2630	O	ILE	B	843	-10.953	9.744	39.101	1.00	43.29
2631	CB	ILE	B	843	-7.752	8.946	38.109	1.00	40.36
2632	CG1	ILE	B	843	-7.767	10.473	37.976	1.00	40.52
2633	CG2	ILE	B	843	-6.99	8.305	36.955	1.00	41.19
2634	CD1	ILE	B	843	-6.42	11.131	38.18	1.00	39.46
2635	N	LYS	B	844	-9.384	8.945	40.499	1.00	45.28
2636	CA	LYS	B	844	-9.977	9.575	41.668	1.00	48.03
2637	C	LYS	B	844	-8.962	10.49	42.33	1.00	49.44
2638	O	LYS	B	844	-8.037	10.021	42.994	1.00	50.39
2639	CB	LYS	B	844	-10.438	8.528	42.678	1.00	49.71
2640	CG	LYS	B	844	-10.934	9.129	43.989	1.00	51.77
2641	CD	LYS	B	844	-11.251	8.047	45.011	1.00	54.31
2642	CE	LYS	B	844	-11.654	8.649	46.348	1.00	55.65
2643	NZ	LYS	B	844	-11.934	7.601	47.372	1.00	57.45
2644	N	LYS	B	845	-9.128	11.794	42.142	1.00	50.04
2645	CA	LYS	B	845	-8.223	12.752	42.756	1.00	51.44
2646	C	LYS	B	845	-9.014	13.784	43.548	1.00	51.77
2647	O	LYS	B	845	-9.996	14.338	43.056	1.00	52.09
2648	CB	LYS	B	845	-7.365	13.447	41.696	1.00	52.06
2649	CG	LYS	B	845	-6.311	14.362	42.3	1.00	53.77
2650	CD	LYS	B	845	-5.309	14.871	41.272	1.00	54.11
2651	CE	LYS	B	845	-4.209	15.668	41.962	1.00	54.45

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

2652	NZ	LYS	B	845	-3.12	16.074	41.036	1.00	55.6
2653	N	ASP	B	846	-8.583	14.026	44.783	1.00	52.33
2654	CA	ASP	B	846	-9.24	14.987	45.664	1.00	52.59
2655	C	ASP	B	846	-10.703	14.623	45.91	1.00	51.59
2656	O	ASP	B	846	-11.561	15.501	46.026	1.00	51.21
2657	CB	ASP	B	846	-9.144	16.399	45.074	1.00	54.09
2658	CG	ASP	B	846	-7.715	16.797	44.751	1.00	55.87
2659	OD1	ASP	B	846	-6.835	16.597	45.615	1.00	56.85
2660	OD2	ASP	B	846	-7.47	17.314	43.638	1.00	57.13
2661	N	GLY	B	847	-10.98	13.325	45.978	1.00	50.97
2662	CA	GLY	B	847	-12.336	12.861	46.225	1.00	49.46
2663	C	GLY	B	847	-13.255	12.87	45.019	1.00	48.7
2664	O	GLY	B	847	-14.387	12.392	45.097	1.00	48.43
2665	N	LEU	B	848	-12.775	13.402	43.899	1.00	47.6
2666	CA	LEU	B	848	-13.589	13.465	42.692	1.00	46.78
2667	C	LEU	B	848	-13.111	12.58	41.555	1.00	45.96
2668	O	LEU	B	848	-11.912	12.416	41.328	1.00	45.76
2669	CB	LEU	B	848	-13.67	14.899	42.168	1.00	46.81
2670	CG	LEU	B	848	-14.493	15.909	42.959	1.00	47.95
2671	CD1	LEU	B	848	-14.531	17.232	42.201	1.00	47.55
2672	CD2	LEU	B	848	-15.899	15.369	43.161	1.00	48.37
2673	N	ARG	B	849	-14.074	12.021	40.834	1.00	44.86
2674	CA	ARG	B	849	-13.782	11.187	39.687	1.00	44.3
2675	C	ARG	B	849	-13.616	12.163	38.522	1.00	42.46
2676	O	ARG	B	849	-14.513	12.949	38.23	1.00	42.82
2677	CB	ARG	B	849	-14.942	10.224	39.43	1.00	45.28
2678	CG	ARG	B	849	-15.242	9.301	40.61	1.00	48.04
2679	CD	ARG	B	849	-15.033	7.846	40.229	1.00	49.46
2680	NE	ARG	B	849	-13.656	7.597	39.812	1.00	51.98
2681	CZ	ARG	B	849	-13.268	6.546	39.096	1.00	52.47
2682	NH1	ARG	B	849	-14.152	5.637	38.71	1.00	53.63
2683	NH2	ARG	B	849	-11.997	6.412	38.753	1.00	51.9
2684	N	MET	B	850	-12.459	12.122	37.873	1.00	40.39
2685	CA	MET	B	850	-12.181	13.019	36.762	1.00	38.66
2686	C	MET	B	850	-11.579	12.304	35.557	1.00	37.1
2687	O	MET	B	850	-11.134	11.16	35.651	1.00	36.71
2688	CB	MET	B	850	-11.221	14.12	37.215	1.00	39.54
2689	CG	MET	B	850	-9.898	13.59	37.76	1.00	41.32
2690	SD	MET	B	850	-8.621	14.858	37.924	1.00	42.82

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

2691	CE	MET	B	850	-8.96	15.481	39.568	1.00	45.17
2692	N	ASP	B	851	-11.578	12.996	34.424	1.00	35.14
2693	CA	ASP	B	851	-11.01	12.472	33.19	1.00	33.54
2694	C	ASP	B	851	-9.497	12.618	33.231	1.00	31.6
2695	O	ASP	B	851	-8.967	13.582	33.785	1.00	30.69
2696	CB	ASP	B	851	-11.538	13.251	31.988	1.00	34.79
2697	CG	ASP	B	851	-12.966	12.905	31.651	1.00	36.35
2698	OD1	ASP	B	851	-13.62	13.723	30.972	1.00	37.96
2699	OD2	ASP	B	851	-13.427	11.817	32.052	1.00	37.14
2700	N	ALA	B	852	-8.805	11.658	32.636	1.00	30.36
2701	CA	ALA	B	852	-7.355	11.697	32.585	1.00	28.54
2702	C	ALA	B	852	-6.881	10.709	31.547	1.00	27.41
2703	O	ALA	B	852	-7.681	10.004	30.937	1.00	27.67
2704	CB	ALA	B	852	-6.76	11.353	33.948	1.00	28.71
2705	N	ALA	B	853	-5.574	10.687	31.332	1.00	26.22
2706	CA	ALA	B	853	-4.963	9.764	30.397	1.00	25.8
2707	C	ALA	B	853	-3.889	9.073	31.221	1.00	26.05
2708	O	ALA	B	853	-3.366	9.653	32.172	1.00	26.24
2709	CB	ALA	B	853	-4.343	10.517	29.232	1.00	25.81
2710	N	ILE	B	854	-3.561	7.839	30.876	1.00	25.34
2711	CA	ILE	B	854	-2.55	7.134	31.634	1.00	25.73
2712	C	ILE	B	854	-1.42	6.593	30.776	1.00	26.38
2713	O	ILE	B	854	-1.637	5.848	29.812	1.00	23.07
2714	CB	ILE	B	854	-3.197	6.002	32.467	1.00	28.19
2715	CG1	ILE	B	854	-4.01	6.632	33.607	1.00	29.19
2716	CG2	ILE	B	854	-2.13	5.067	33.025	1.00	27.76
2717	CD1	ILE	B	854	-4.735	5.648	34.48	1.00	31.9
2718	N	LYS	B	855	-0.207	7	31.14	1.00	27.08
2719	CA	LYS	B	855	1.001	6.582	30.451	1.00	28.41
2720	C	LYS	B	855	1.632	5.448	31.236	1.00	29.65
2721	O	LYS	B	855	2.104	5.637	32.356	1.00	29.33
2722	CB	LYS	B	855	1.988	7.746	30.353	1.00	28.5
2723	CG	LYS	B	855	3.361	7.363	29.805	1.00	28.85
2724	CD	LYS	B	855	3.27	6.812	28.394	1.00	27.85
2725	CE	LYS	B	855	4.656	6.59	27.814	1.00	27.94
2726	NZ	LYS	B	855	4.595	6.112	26.406	1.00	28
2727	N	ARG	B	856	1.639	4.271	30.627	1.00	31.7
2728	CA	ARG	B	856	2.196	3.072	31.228	1.00	33.23
2729	C	ARG	B	856	3.699	2.996	30.966	1.00	34.32

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

2730	O	ARG	B	856	4.137	2.914	29.82	1.00	33.86
2731	CB	ARG	B	856	1.47	1.86	30.643	1.00	34.28
2732	CG	ARG	B	856	1.829	0.524	31.245	1.00	36.9
2733	CD	ARG	B	856	0.707	-0.455	30.986	1.00	38.4
2734	NE	ARG	B	856	1.053	-1.821	31.355	1.00	40.51
2735	CZ	ARG	B	856	1.776	-2.638	30.599	1.00	41.03
2736	NH1	ARG	B	856	2.239	-2.227	29.425	1.00	41.23
2737	NH2	ARG	B	856	2.022	-3.872	31.01	1.00	42.28
2738	N	MET	B	857	4.484	3.029	32.039	1.00	36.38
2739	CA	MET	B	857	5.94	2.98	31.937	1.00	38.62
2740	C	MET	B	857	6.522	1.702	32.535	1.00	40.68
2741	O	MET	B	857	6.334	1.414	33.72	1.00	40.63
2742	CB	MET	B	857	6.554	4.197	32.642	1.00	37.7
2743	CG	MET	B	857	6.248	5.532	31.972	1.00	38.1
2744	SD	MET	B	857	6.649	6.976	32.985	1.00	37.71
2745	CE	MET	B	857	8.444	7.006	32.865	1.00	36.78
2746	N	ALA	B	858	7.229	0.932	31.713	1.00	43.46
2747	CA	ALA	B	858	7.85	-0.303	32.185	1.00	46.4
2748	C	ALA	B	858	9.007	0.101	33.095	1.00	47.81
2749	O	ALA	B	858	9.839	0.926	32.716	1.00	47.44
2750	CB	ALA	B	858	8.362	-1.127	31	1.00	46.55
2751	N	GLU	B	859	9.057	-0.471	34.293	1.00	49.89
2752	CA	GLU	B	859	10.11	-0.131	35.241	1.00	52.79
2753	C	GLU	B	859	11.4	-0.936	35.09	1.00	54.48
2754	O	GLU	B	859	12.494	-0.395	35.263	1.00	54.7
2755	CB	GLU	B	859	9.577	-0.248	36.671	1.00	52.79
2756	CG	GLU	B	859	8.473	0.752	36.978	1.00	54.12
2757	CD	GLU	B	859	7.991	0.686	38.411	1.00	54.99
2758	OE1	GLU	B	859	7.48	-0.378	38.816	1.00	55.69
2759	OE2	GLU	B	859	8.121	1.701	39.132	1.00	55.74
2760	N	ALA	B	860	11.28	-2.219	34.761	1.00	56.18
2761	CA	ALA	B	860	12.46	-3.066	34.596	1.00	57.56
2762	C	ALA	B	860	12.819	-3.261	33.124	1.00	58.2
2763	OT1	ALA	B	860	13.862	-2.721	32.692	1.00	58.48
2764	CB	ALA	B	860	12.227	-4.416	35.262	1.00	57.38
2765	OT2	ALA	B	860	12.052	-3.947	32.416	1.00	58.76
2766	N	ALA	B	867	19.141	3.886	35.403	1.00	68.56
2767	CA	ALA	B	867	18.187	3.262	34.44	1.00	68.13
2768	C	ALA	B	867	17.668	4.285	33.435	1.00	67.81

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

2769	O	ALA	B	867	17.894	5.489	33.576	1.00	67.71
2770	CB	ALA	B	867	17.012	2.633	35.197	1.00	67.85
2771	N	ASP	B	868	16.975	3.79	32.415	1.00	67.24
2772	CA	ASP	B	868	16.401	4.636	31.378	1.00	66.33
2773	C	ASP	B	868	15.059	5.146	31.906	1.00	65.18
2774	O	ASP	B	868	14.589	6.223	31.534	1.00	64.6
2775	CB	ASP	B	868	16.196	3.811	30.106	1.00	67.74
2776	CG	ASP	B	868	15.858	4.66	28.904	1.00	68.95
2777	OD1	ASP	B	868	14.783	5.3	28.909	1.00	70.59
2778	OD2	ASP	B	868	16.671	4.687	27.952	1.00	69.38
2779	N	PHE	B	869	14.465	4.348	32.79	1.00	63.8
2780	CA	PHE	B	869	13.184	4.65	33.42	1.00	61.71
2781	C	PHE	B	869	13.36	5.706	34.51	1.00	60.75
2782	O	PHE	B	869	12.645	6.708	34.538	1.00	60.51
2783	CB	PHE	B	869	12.604	3.369	34.029	1.00	61.02
2784	CG	PHE	B	869	11.425	3.598	34.93	1.00	60.3
2785	CD1	PHE	B	869	10.188	3.954	34.407	1.00	60.3
2786	CD2	PHE	B	869	11.557	3.468	36.308	1.00	60.18
2787	CE1	PHE	B	869	9.096	4.18	35.245	1.00	60.28
2788	CE2	PHE	B	869	10.472	3.691	37.157	1.00	60.46
2789	CZ	PHE	B	869	9.239	4.048	36.624	1.00	60.08
2790	N	ALA	B	870	14.317	5.472	35.404	1.00	59.69
2791	CA	ALA	B	870	14.591	6.391	36.506	1.00	58.58
2792	C	ALA	B	870	14.988	7.778	36.006	1.00	57.31
2793	O	ALA	B	870	14.682	8.786	36.642	1.00	57.29
2794	CB	ALA	B	870	15.692	5.823	37.4	1.00	57.92
2795	N	GLY	B	871	15.675	7.821	34.87	1.00	55.95
2796	CA	GLY	B	871	16.096	9.091	34.308	1.00	54.5
2797	C	GLY	B	871	14.919	9.918	33.826	1.00	53.44
2798	O	GLY	B	871	14.848	11.117	34.089	1.00	52.87
2799	N	GLU	B	872	13.992	9.275	33.122	1.00	52.24
2800	CA	GLU	B	872	12.817	9.96	32.608	1.00	51.98
2801	C	GLU	B	872	11.886	10.364	33.741	1.00	51.04
2802	O	GLU	B	872	11.159	11.353	33.642	1.00	50.47
2803	CB	GLU	B	872	12.073	9.063	31.618	1.00	53.17
2804	CG	GLU	B	872	12.88	8.749	30.367	1.00	55.87
2805	CD	GLU	B	872	12.078	8.002	29.317	1.00	57.04
2806	OE1	GLU	B	872	11.544	6.918	29.634	1.00	56.82
2807	OE2	GLU	B	872	11.986	8.502	28.172	1.00	58.13

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

2808	N	LEU	B	873	11.919	9.597	34.822	1.00	50.02
2809	CA	LEU	B	873	11.075	9.867	35.978	1.00	49.52
2810	C	LEU	B	873	11.615	11.068	36.752	1.00	48.72
2811	O	LEU	B	873	10.851	11.87	37.291	1.00	47.77
2812	CB	LEU	B	873	11.023	8.625	36.876	1.00	50.48
2813	CG	LEU	B	873	10.002	8.549	38.015	1.00	51.45
2814	CD1	LEU	B	873	9.923	7.121	38.533	1.00	51.64
2815	CD2	LEU	B	873	10.394	9.499	39.133	1.00	52.61
2816	N	GLU	B	874	12.937	11.194	36.792	1.00	47.93
2817	CA	GLU	B	874	13.574	12.296	37.498	1.00	47.18
2818	C	GLU	B	874	13.252	13.629	36.829	1.00	45.01
2819	O	GLU	B	874	13.117	14.655	37.498	1.00	43.85
2820	CB	GLU	B	874	15.091	12.095	37.546	1.00	49.92
2821	CG	GLU	B	874	15.784	13.049	38.502	1.00	54.32
2822	CD	GLU	B	874	15.169	12.999	39.895	1.00	56.99
2823	OE1	GLU	B	874	15.204	11.917	40.524	1.00	58.51
2824	OE2	GLU	B	874	14.644	14.039	40.358	1.00	58.39
2825	N	VAL	B	875	13.135	13.612	35.505	1.00	42.89
2826	CA	VAL	B	875	12.812	14.827	34.768	1.00	40.15
2827	C	VAL	B	875	11.353	15.206	35.005	1.00	39.59
2828	O	VAL	B	875	11.04	16.372	35.241	1.00	38.03
2829	CB	VAL	B	875	13.035	14.646	33.257	1.00	39.71
2830	CG1	VAL	B	875	12.65	15.92	32.52	1.00	37.59
2831	CG2	VAL	B	875	14.49	14.292	32.986	1.00	38.62
2832	N	LEU	B	876	10.468	14.212	34.954	1.00	39.12
2833	CA	LEU	B	876	9.037	14.432	35.154	1.00	39.23
2834	C	LEU	B	876	8.706	15.078	36.498	1.00	39.9
2835	O	LEU	B	876	7.84	15.954	36.576	1.00	39.76
2836	CB	LEU	B	876	8.269	13.109	35.028	1.00	38.06
2837	CG	LEU	B	876	8.196	12.425	33.658	1.00	38.21
2838	CD1	LEU	B	876	7.547	11.053	33.805	1.00	37.95
2839	CD2	LEU	B	876	7.4	13.287	32.685	1.00	36.94
2840	N	CYS	B	877	9.389	14.646	37.553	1.00	40.35
2841	CA	CYS	B	877	9.149	15.182	38.891	1.00	41.4
2842	C	CYS	B	877	9.534	16.649	39.034	1.00	40.88
2843	O	CYS	B	877	9.11	17.321	39.976	1.00	40.97
2844	CB	CYS	B	877	9.905	14.358	39.937	1.00	43.15
2845	SG	CYS	B	877	9.207	12.717	40.219	1.00	48.4
2846	N	LYS	B	878	10.337	17.145	38.102	1.00	40.12



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TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

2847	CA	LYS	B	878	10.766	18.532	38.15	1.00	39.54
2848	C	LYS	B	878	9.89	19.439	37.286	1.00	37.92
2849	O	LYS	B	878	10.141	20.639	37.196	1.00	38.25
2850	CB	LYS	B	878	12.229	18.633	37.719	1.00	41.67
2851	CG	LYS	B	878	13.145	17.818	38.62	1.00	45.36
2852	CD	LYS	B	878	14.623	18.081	38.379	1.00	48.97
2853	CE	LYS	B	878	15.465	17.313	39.405	1.00	51.18
2854	NZ	LYS	B	878	16.935	17.521	39.239	1.00	53.87
2855	N	LEU	B	879	8.852	18.865	36.696	1.00	35.88
2856	CA	LEU	B	879	7.946	19.634	35.852	1.00	34.85
2857	C	LEU	B	879	7.146	20.664	36.641	1.00	33.99
2858	O	LEU	B	879	6.947	21.784	36.182	1.00	34.35
2859	CB	LEU	B	879	6.978	18.707	35.108	1.00	33.03
2860	CG	LEU	B	879	7.496	17.948	33.882	1.00	32.84
2861	CD1	LEU	B	879	6.388	17.06	33.326	1.00	32.07
2862	CD2	LEU	B	879	7.964	18.933	32.825	1.00	31.76
2863	N	GLY	B	880	6.692	20.291	37.829	1.00	33.45
2864	CA	GLY	B	880	5.908	21.221	38.616	1.00	33.19
2865	C	GLY	B	880	4.546	21.365	37.97	1.00	33.82
2866	O	GLY	B	880	4.082	20.443	37.297	1.00	34.84
2867	N	HIS	B	881	3.9	22.511	38.159	1.00	32.57
2868	CA	HIS	B	881	2.588	22.736	37.569	1.00	32.58
2869	C	HIS	B	881	2.458	24.078	36.867	1.00	30.83
2870	O	HIS	B	881	2.992	25.091	37.324	1.00	29.92
2871	CB	HIS	B	881	1.491	22.618	38.627	1.00	34.76
2872	CG	HIS	B	881	1.192	21.209	39.023	1.00	39.71
2873	ND1	HIS	B	881	1.902	20.542	39.999	1.00	42.4
2874	CD2	HIS	B	881	0.288	20.324	38.542	1.00	41.25
2875	CE1	HIS	B	881	1.447	19.306	40.101	1.00	43.37
2876	NE2	HIS	B	881	0.466	19.148	39.229	1.00	43.38
2877	N	HIS	B	882	1.742	24.064	35.748	1.00	27.47
2878	CA	HIS	B	882	1.503	25.26	34.955	1.00	25.87
2879	C	HIS	B	882	0.338	24.983	34.022	1.00	24.57
2880	O	HIS	B	882	0.214	23.888	33.485	1.00	24.57
2881	CB	HIS	B	882	2.745	25.634	34.148	1.00	23.76
2882	CG	HIS	B	882	2.65	26.979	33.507	1.00	23.64
2883	ND1	HIS	B	882	1.926	27.207	32.356	1.00	23.3
2884	CD2	HIS	B	882	3.137	28.182	33.891	1.00	22.69
2885	CE1	HIS	B	882	1.97	28.493	32.061	1.00	22.82

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

2886	NE2	HIS	B	882	2.697	29.106	32.977	1.00	22.83
2887	N	PRO	B	883	-0.538	25.975	33.819	1.00	24.54
2888	CA	PRO	B	883	-1.705	25.819	32.944	1.00	23.69
2889	C	PRO	B	883	-1.375	25.438	31.498	1.00	22.44
2890	O	PRO	B	883	-2.164	24.764	30.839	1.00	21.9
2891	CB	PRO	B	883	-2.385	27.192	33.016	1.00	23.86
2892	CG	PRO	B	883	-1.953	27.728	34.335	1.00	26.19
2893	CD	PRO	B	883	-0.502	27.327	34.4	1.00	24.73
2894	N	ASN	B	884	-0.215	25.856	31.007	1.00	20.66
2895	CA	ASN	B	884	0.127	25.568	29.619	1.00	20.88
2896	C	ASN	B	884	1.083	24.397	29.355	1.00	20.97
2897	O	ASN	B	884	1.815	24.387	28.361	1.00	20.08
2898	CB	ASN	B	884	0.629	26.85	28.944	1.00	19.99
2899	CG	ASN	B	884	-0.38	28.002	29.054	1.00	21.26
2900	OD1	ASN	B	884	-0.071	29.064	29.597	1.00	21.05
2901	ND2	ASN	B	884	-1.589	27.786	28.545	1.00	18.98
2902	N	ILE	B	885	1.091	23.421	30.258	1.00	21.45
2903	CA	ILE	B	885	1.893	22.212	30.058	1.00	22.46
2904	C	ILE	B	885	0.968	21.081	30.463	1.00	22.82
2905	O	ILE	B	885	-0.053	21.329	31.094	1.00	23.11
2906	CB	ILE	B	885	3.156	22.122	30.96	1.00	21.98
2907	CG1	ILE	B	885	2.749	21.985	32.43	1.00	22.03
2908	CG2	ILE	B	885	4.075	23.311	30.715	1.00	21.71
2909	CD1	ILE	B	885	3.901	21.556	33.337	1.00	22.46
2910	N	ILE	B	886	1.296	19.851	30.084	1.00	23.26
2911	CA	ILE	B	886	0.469	18.722	30.497	1.00	23.22
2912	C	ILE	B	886	0.891	18.443	31.938	1.00	22.57
2913	O	ILE	B	886	2.048	18.116	32.207	1.00	21.88
2914	CB	ILE	B	886	0.716	17.473	29.615	1.00	22.72
2915	CG1	ILE	B	886	0.171	17.719	28.202	1.00	22.97
2916	CG2	ILE	B	886	0.072	16.231	30.258	1.00	19.41
2917	CD1	ILE	B	886	-1.336	17.921	28.125	1.00	22.62
2918	N	ASN	B	887	-0.044	18.601	32.863	1.00	23.68
2919	CA	ASN	B	887	0.241	18.39	34.278	1.00	25.98
2920	C	ASN	B	887	0.062	16.941	34.708	1.00	27.09
2921	O	ASN	B	887	-0.823	16.244	34.224	1.00	25.49
2922	CB	ASN	B	887	-0.649	19.306	35.13	1.00	26.59
2923	CG	ASN	B	887	-0.281	20.773	34.982	1.00	28.28
2924	OD1	ASN	B	887	0.751	21.224	35.49	1.00	29.08

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

2925	ND2	ASN	B	887	-1.112	21.521	34.266	1.00	28.67
2926	N	LEU	B	888	0.925	16.495	35.616	1.00	29.44
2927	CA	LEU	B	888	0.867	15.134	36.129	1.00	31.3
2928	C	LEU	B	888	-0.166	15.113	37.249	1.00	32.25
2929	O	LEU	B	888	-0.135	15.954	38.142	1.00	33.55
2930	CB	LEU	B	888	2.241	14.718	36.653	1.00	32.07
2931	CG	LEU	B	888	3.403	14.987	35.687	1.00	33.16
2932	CD1	LEU	B	888	4.677	14.374	36.242	1.00	33.67
2933	CD2	LEU	B	888	3.088	14.405	34.31	1.00	32.25
2934	N	LEU	B	889	-1.082	14.154	37.197	1.00	33.15
2935	CA	LEU	B	889	-2.14	14.064	38.191	1.00	34.62
2936	C	LEU	B	889	-1.877	13.045	39.293	1.00	36.02
2937	O	LEU	B	889	-2.634	12.962	40.258	1.00	37.13
2938	CB	LEU	B	889	-3.465	13.739	37.498	1.00	33.75
2939	CG	LEU	B	889	-3.852	14.69	36.36	1.00	34.36
2940	CD1	LEU	B	889	-5.192	14.27	35.772	1.00	33.22
2941	CD2	LEU	B	889	-3.927	16.118	36.89	1.00	33.86
2942	N	GLY	B	890	-0.797	12.285	39.152	1.00	37.31
2943	CA	GLY	B	890	-0.461	11.27	40.136	1.00	37.67
2944	C	GLY	B	890	0.043	10.015	39.445	1.00	38.56
2945	O	GLY	B	890	0.132	9.972	38.221	1.00	38.7
2946	N	ALA	B	891	0.377	8.99	40.219	1.00	39.91
2947	CA	ALA	B	891	0.875	7.747	39.641	1.00	40.48
2948	C	ALA	B	891	0.495	6.536	40.485	1.00	40.99
2949	O	ALA	B	891	0.088	6.671	41.639	1.00	40.46
2950	CB	ALA	B	891	2.385	7.817	39.477	1.00	39.65
2951	N	CYS	B	892	0.636	5.352	39.892	1.00	41.6
2952	CA	CYS	B	892	0.307	4.103	40.56	1.00	42.26
2953	C	CYS	B	892	1.156	2.953	40.033	1.00	43.36
2954	O	CYS	B	892	1.166	2.693	38.831	1.00	42.97
2955	CB	CYS	B	892	-1.167	3.777	40.344	1.00	41.74
2956	SG	CYS	B	892	-1.635	2.127	40.891	1.00	42.71
2957	N	GLU	B	893	1.87	2.269	40.928	1.00	44.44
2958	CA	GLU	B	893	2.697	1.132	40.524	1.00	45.65
2959	C	GLU	B	893	1.844	-0.125	40.546	1.00	45.26
2960	O	GLU	B	893	1.165	-0.403	41.534	1.00	45.88
2961	CB	GLU	B	893	3.891	0.952	41.461	1.00	47.28
2962	CG	GLU	B	893	4.973	2.004	41.304	1.00	51.06
2963	CD	GLU	B	893	6.222	1.676	42.104	1.00	53.64

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

2964	OE1	GLU	B	893	6.889	0.668	41.777	1.00	55.49
2965	OE2	GLU	B	893	6.531	2.419	43.062	1.00	54.34
2966	N	HIS	B	894	1.882	-0.885	39.456	1.00	44.44
2967	CA	HIS	B	894	1.084	-2.103	39.348	1.00	43.56
2968	C	HIS	B	894	1.78	-3.144	38.474	1.00	43.13
2969	O	HIS	B	894	2.029	-2.91	37.292	1.00	41.35
2970	CB	HIS	B	894	-0.283	-1.758	38.752	1.00	42.6
2971	CG	HIS	B	894	-1.256	-2.896	38.745	1.00	42.55
2972	ND1	HIS	B	894	-1.857	-3.371	39.89	1.00	42.11
2973	CD2	HIS	B	894	-1.774	-3.617	37.721	1.00	41.96
2974	CE1	HIS	B	894	-2.706	-4.331	39.572	1.00	42.08
2975	NE2	HIS	B	894	-2.676	-4.499	38.262	1.00	41.64
2976	N	ALA	B	895	2.1	-4.286	39.077	1.00	43.16
2977	CA	ALA	B	895	2.752	-5.393	38.384	1.00	43.24
2978	C	ALA	B	895	4.031	-5.021	37.637	1.00	43.58
2979	O	ALA	B	895	4.242	-5.464	36.509	1.00	44.21
2980	CB	ALA	B	895	1.762	-6.051	37.423	1.00	42.52
2981	N	GLY	B	896	4.882	-4.213	38.261	1.00	43.78
2982	CA	GLY	B	896	6.137	-3.832	37.63	1.00	44.34
2983	C	GLY	B	896	6.051	-2.706	36.613	1.00	45.04
2984	O	GLY	B	896	7.019	-2.404	35.911	1.00	44.93
2985	N	TYR	B	897	4.888	-2.078	36.531	1.00	44.8
2986	CA	TYR	B	897	4.684	-0.979	35.599	1.00	44.4
2987	C	TYR	B	897	4.18	0.245	36.354	1.00	43.08
2988	O	TYR	B	897	3.347	0.133	37.255	1.00	42.76
2989	CB	TYR	B	897	3.656	-1.373	34.537	1.00	45.79
2990	CG	TYR	B	897	4.144	-2.363	33.501	1.00	47.31
2991	CD1	TYR	B	897	4.677	-1.927	32.287	1.00	47.8
2992	CD2	TYR	B	897	4.038	-3.734	33.719	1.00	48.12
2993	CE1	TYR	B	897	5.085	-2.838	31.31	1.00	48.51
2994	CE2	TYR	B	897	4.444	-4.652	32.753	1.00	48.4
2995	CZ	TYR	B	897	4.963	-4.2	31.55	1.00	49.14
2996	OH	TYR	B	897	5.335	-5.116	30.583	1.00	50.2
2997	N	LEU	B	898	4.696	1.414	36.001	1.00	41.81
2998	CA	LEU	B	898	4.244	2.634	36.646	1.00	39.91
2999	C	LEU	B	898	3.148	3.224	35.77	1.00	38.32
3000	O	LEU	B	898	3.358	3.474	34.582	1.00	38.69
3001	CB	LEU	B	898	5.39	3.637	36.794	1.00	40.78
3002	CG	LEU	B	898	5.005	4.955	37.481	1.00	41.82

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

3003	CD1	LEU	B	898	4.578	4.689	38.915	1.00	42.01
3004	CD2	LEU	B	898	6.185	5.911	37.452	1.00	42.85
3005	N	TYR	B	899	1.968	3.415	36.346	1.00	35.56
3006	CA	TYR	B	899	0.856	3.991	35.608	1.00	33.27
3007	C	TYR	B	899	0.761	5.477	35.939	1.00	33.27
3008	O	TYR	B	899	0.154	5.871	36.937	1.00	34.3
3009	CB	TYR	B	899	-0.44	3.267	35.963	1.00	31.19
3010	CG	TYR	B	899	-0.532	1.876	35.371	1.00	31.26
3011	CD1	TYR	B	899	-1.371	1.611	34.29	1.00	30.94
3012	CD2	TYR	B	899	0.241	0.827	35.876	1.00	31.18
3013	CE1	TYR	B	899	-1.442	0.34	33.725	1.00	30.75
3014	CE2	TYR	B	899	0.179	-0.449	35.316	1.00	30.92
3015	CZ	TYR	B	899	-0.664	-0.684	34.244	1.00	31.2
3016	OH	TYR	B	899	-0.73	-1.94	33.688	1.00	32.57
3017	N	LEU	B	900	1.381	6.292	35.094	1.00	31.28
3018	CA	LEU	B	900	1.401	7.737	35.273	1.00	30.42
3019	C	LEU	B	900	0.126	8.403	34.756	1.00	28.47
3020	O	LEU	B	900	-0.206	8.285	33.576	1.00	28.92
3021	CB	LEU	B	900	2.615	8.322	34.543	1.00	30.23
3022	CG	LEU	B	900	2.876	9.821	34.709	1.00	31.99
3023	CD1	LEU	B	900	3.258	10.103	36.164	1.00	31.83
3024	CD2	LEU	B	900	3.99	10.269	33.762	1.00	30.52
3025	N	ALA	B	901	-0.593	9.092	35.64	1.00	26.24
3026	CA	ALA	B	901	-1.815	9.788	35.239	1.00	26.06
3027	C	ALA	B	901	-1.463	11.214	34.827	1.00	25.62
3028	O	ALA	B	901	-0.727	11.903	35.535	1.00	25.85
3029	CB	ALA	B	901	-2.811	9.818	36.379	1.00	25.11
3030	N	ILE	B	902	-1.979	11.644	33.678	1.00	24.36
3031	CA	ILE	B	902	-1.724	12.99	33.175	1.00	24.78
3032	C	ILE	B	902	-3.027	13.621	32.699	1.00	25.18
3033	O	ILE	B	902	-4.043	12.938	32.57	1.00	25.25
3034	CB	ILE	B	902	-0.706	12.975	32.005	1.00	23.45
3035	CG1	ILE	B	902	-1.318	12.311	30.774	1.00	21.03
3036	CG2	ILE	B	902	0.542	12.204	32.419	1.00	24.32
3037	CD1	ILE	B	902	-0.369	12.253	29.599	1.00	20.62
3038	N	GLU	B	903	-2.998	14.925	32.446	1.00	26.38
3039	CA	GLU	B	903	-4.191	15.638	31.993	1.00	28.07
3040	C	GLU	B	903	-4.697	15.134	30.655	1.00	28.37
3041	O	GLU	B	903	-3.916	14.841	29.744	1.00	28.67

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TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

3042	CB	GLU	B	903	-3.922	17.138	31.865	1.00	29.56
3043	CG	GLU	B	903	-3.877	17.899	33.166	1.00	31.23
3044	CD	GLU	B	903	-3.61	19.373	32.943	1.00	32.45
3045	OE1	GLU	B	903	-2.572	19.694	32.329	1.00	32.25
3046	OE2	GLU	B	903	-4.435	20.206	33.376	1.00	33.38
3047	N	TYR	B	904	-6.015	15.045	30.546	1.00	28.16
3048	CA	TYR	B	904	-6.648	14.603	29.32	1.00	28.23
3049	C	TYR	B	904	-7.039	15.825	28.486	1.00	28.73
3050	O	TYR	B	904	-7.667	16.757	28.992	1.00	28.96
3051	CB	TYR	B	904	-7.893	13.775	29.647	1.00	27.17
3052	CG	TYR	B	904	-8.799	13.546	28.459	1.00	27.35
3053	CD1	TYR	B	904	-8.371	12.794	27.365	1.00	27.61
3054	CD2	TYR	B	904	-10.079	14.096	28.422	1.00	27.81
3055	CE1	TYR	B	904	-9.198	12.596	26.262	1.00	28.9
3056	CE2	TYR	B	904	-10.911	13.907	27.327	1.00	28.51
3057	CZ	TYR	B	904	-10.465	13.155	26.249	1.00	29.52
3058	OH	TYR	B	904	-11.287	12.973	25.158	1.00	31.72
3059	N	ALA	B	905	-6.659	15.815	27.211	1.00	28.39
3060	CA	ALA	B	905	-6.98	16.907	26.293	1.00	28.44
3061	C	ALA	B	905	-8.164	16.477	25.423	1.00	28.43
3062	O	ALA	B	905	-8.024	15.638	24.534	1.00	28.71
3063	CB	ALA	B	905	-5.765	17.229	25.42	1.00	28.22
3064	N	PRO	B	906	-9.35	17.05	25.676	1.00	28.36
3065	CA	PRO	B	906	-10.607	16.77	24.962	1.00	28.44
3066	C	PRO	B	906	-10.606	17.082	23.466	1.00	28.64
3067	O	PRO	B	906	-11.396	16.516	22.709	1.00	28.93
3068	CB	PRO	B	906	-11.632	17.647	25.692	1.00	28.5
3069	CG	PRO	B	906	-11.016	17.879	27.043	1.00	29.97
3070	CD	PRO	B	906	-9.559	18.065	26.72	1.00	28.67
3071	N	HIS	B	907	-9.732	17.989	23.042	1.00	28.29
3072	CA	HIS	B	907	-9.693	18.391	21.643	1.00	27.5
3073	C	HIS	B	907	-8.484	17.892	20.851	1.00	26.84
3074	O	HIS	B	907	-8.173	18.423	19.78	1.00	25.39
3075	CB	HIS	B	907	-9.789	19.916	21.569	1.00	27.83
3076	CG	HIS	B	907	-10.929	20.478	22.356	1.00	29.27
3077	ND1	HIS	B	907	-12.247	20.259	22.014	1.00	31.12
3078	CD2	HIS	B	907	-10.953	21.2	23.501	1.00	30.15
3079	CE1	HIS	B	907	-13.033	20.822	22.917	1.00	31.41
3080	NE2	HIS	B	907	-12.272	21.397	23.83	1.00	31.16

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

3081	N	GLY	B	908	-7.809	16.87	21.371	1.00	25.66
3082	CA	GLY	B	908	-6.657	16.318	20.674	1.00	25.02
3083	C	GLY	B	908	-5.484	17.272	20.503	1.00	24.42
3084	O	GLY	B	908	-5.405	18.299	21.176	1.00	24.08
3085	N	ASN	B	909	-4.571	16.939	19.595	1.00	24.37
3086	CA	ASN	B	909	-3.404	17.778	19.366	1.00	24.47
3087	C	ASN	B	909	-3.741	18.975	18.479	1.00	24
3088	O	ASN	B	909	-4.706	18.948	17.709	1.00	23.89
3089	CB	ASN	B	909	-2.265	16.952	18.76	1.00	25.39
3090	CG	ASN	B	909	-2.523	16.564	17.316	1.00	26.84
3091	OD1	ASN	B	909	-2.405	17.388	16.407	1.00	26.77
3092	ND2	ASN	B	909	-2.879	15.305	17.098	1.00	26.75
3093	N	LEU	B	910	-2.932	20.021	18.6	1.00	22.74
3094	CA	LEU	B	910	-3.126	21.266	17.87	1.00	22.18
3095	C	LEU	B	910	-3.09	21.191	16.337	1.00	22.35
3096	O	LEU	B	910	-3.867	21.875	15.668	1.00	20.34
3097	CB	LEU	B	910	-2.102	22.298	18.359	1.00	20.24
3098	CG	LEU	B	910	-2.161	23.691	17.736	1.00	20.88
3099	CD1	LEU	B	910	-3.524	24.339	17.994	1.00	18.07
3100	CD2	LEU	B	910	-1.035	24.543	18.33	1.00	19.98
3101	N	LEU	B	911	-2.192	20.38	15.781	1.00	22.04
3102	CA	LEU	B	911	-2.092	20.269	14.327	1.00	22.91
3103	C	LEU	B	911	-3.419	19.8	13.742	1.00	22.96
3104	O	LEU	B	911	-3.966	20.412	12.826	1.00	21.9
3105	CB	LEU	B	911	-0.985	19.288	13.934	1.00	22.01
3106	CG	LEU	B	911	-0.709	19.151	12.43	1.00	21.69
3107	CD1	LEU	B	911	-0.354	20.515	11.841	1.00	22.01
3108	CD2	LEU	B	911	0.431	18.173	12.208	1.00	19.98
3109	N	ASP	B	912	-3.935	18.712	14.291	1.00	24.16
3110	CA	ASP	B	912	-5.195	18.158	13.83	1.00	26.41
3111	C	ASP	B	912	-6.316	19.178	14.044	1.00	25.69
3112	O	ASP	B	912	-7.2	19.331	13.2	1.00	26.27
3113	CB	ASP	B	912	-5.492	16.859	14.587	1.00	29.04
3114	CG	ASP	B	912	-6.794	16.218	14.159	1.00	34.58
3115	OD1	ASP	B	912	-6.886	15.759	12.999	1.00	38.98
3116	OD2	ASP	B	912	-7.735	16.175	14.982	1.00	37.82
3117	N	PHE	B	913	-6.262	19.892	15.164	1.00	24.6
3118	CA	PHE	B	913	-7.279	20.89	15.481	1.00	24.16
3119	C	PHE	B	913	-7.267	22.025	14.442	1.00	24.02

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TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

3120	O	PHE	B	913	-8.316	22.439	13.946	1.00	23.68
3121	CB	PHE	B	913	-7.04	21.444	16.89	1.00	24.56
3122	CG	PHE	B	913	-8.216	22.177	17.458	1.00	26.43
3123	CD1	PHE	B	913	-9.385	21.496	17.776	1.00	26.37
3124	CD2	PHE	B	913	-8.162	23.55	17.673	1.00	27.37
3125	CE1	PHE	B	913	-10.487	22.17	18.303	1.00	27.94
3126	CE2	PHE	B	913	-9.259	24.234	18.2	1.00	28.62
3127	CZ	PHE	B	913	-10.425	23.541	18.517	1.00	28.12
3128	N	LEU	B	914	-6.073	22.517	14.119	1.00	22.53
3129	CA	LEU	B	914	-5.916	23.577	13.128	1.00	23.11
3130	C	LEU	B	914	-6.453	23.142	11.764	1.00	23.81
3131	O	LEU	B	914	-7.155	23.895	11.094	1.00	24.67
3132	CB	LEU	B	914	-4.437	23.948	12.974	1.00	20.64
3133	CG	LEU	B	914	-3.785	24.652	14.166	1.00	21.69
3134	CD1	LEU	B	914	-2.275	24.684	13.96	1.00	19.34
3135	CD2	LEU	B	914	-4.366	26.07	14.317	1.00	15.43
3136	N	ARG	B	915	-6.102	21.927	11.357	1.00	24.25
3137	CA	ARG	B	915	-6.527	21.386	10.068	1.00	25.39
3138	C	ARG	B	915	-8.032	21.17	9.977	1.00	25.46
3139	O	ARG	B	915	-8.633	21.406	8.937	1.00	24.49
3140	CB	ARG	B	915	-5.776	20.079	9.786	1.00	24.45
3141	CG	ARG	B	915	-4.296	20.325	9.527	1.00	25.95
3142	CD	ARG	B	915	-3.516	19.058	9.245	1.00	25.39
3143	NE	ARG	B	915	-2.158	19.391	8.825	1.00	26.2
3144	CZ	ARG	B	915	-1.191	18.502	8.626	1.00	25.1
3145	NH1	ARG	B	915	0.013	18.909	8.243	1.00	24.4
3146	NH2	ARG	B	915	-1.428	17.209	8.811	1.00	24.39
3147	N	LYS	B	916	-8.639	20.73	11.072	1.00	26.62
3148	CA	LYS	B	916	-10.077	20.509	11.101	1.00	27.07
3149	C	LYS	B	916	-10.86	21.823	11.101	1.00	26.38
3150	O	LYS	B	916	-12.077	21.831	10.918	1.00	26.53
3151	CB	LYS	B	916	-10.448	19.678	12.329	1.00	27.35
3152	CG	LYS	B	916	-9.941	18.255	12.26	1.00	31.13
3153	CD	LYS	B	916	-10.366	17.448	13.48	1.00	33.62
3154	CE	LYS	B	916	-10.039	15.97	13.288	1.00	35.7
3155	NZ	LYS	B	916	-10.337	15.163	14.513	1.00	38.88
3156	N	SER	B	917	-10.164	22.937	11.3	1.00	26.03
3157	CA	SER	B	917	-10.831	24.236	11.319	1.00	26.04
3158	C	SER	B	917	-10.989	24.824	9.91	1.00	25.94



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TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

3159	O	SER	B	917	-11.718	25.798	9.72	1.00	23.79
3160	CB	SER	B	917	-10.055	25.218	12.199	1.00	25.79
3161	OG	SER	B	917	-8.883	25.668	11.539	1.00	26.52
3162	N	ARG	B	918	-10.298	24.228	8.937	1.00	26.88
3163	CA	ARG	B	918	-10.35	24.669	7.542	1.00	27.94
3164	C	ARG	B	918	-11.748	24.363	6.994	1.00	29.98
3165	O	ARG	B	918	-11.931	23.453	6.189	1.00	29.67
3166	CB	ARG	B	918	-9.288	23.931	6.719	1.00	26.07
3167	CG	ARG	B	918	-7.864	24.206	7.161	1.00	25.02
3168	CD	ARG	B	918	-6.855	23.58	6.215	1.00	23.22
3169	NE	ARG	B	918	-5.507	24.089	6.474	1.00	23.29
3170	CZ	ARG	B	918	-4.463	23.879	5.68	1.00	21.36
3171	NH1	ARG	B	918	-3.278	24.378	5.996	1.00	19
3172	NH2	ARG	B	918	-4.607	23.174	4.566	1.00	19.3
3173	N	VAL	B	919	-12.722	25.144	7.446	1.00	31.86
3174	CA	VAL	B	919	-14.119	24.971	7.083	1.00	34.2
3175	C	VAL	B	919	-14.418	25.071	5.586	1.00	35.27
3176	O	VAL	B	919	-15.422	24.551	5.107	1.00	35.42
3177	CB	VAL	B	919	-14.99	25.975	7.888	1.00	34.01
3178	CG1	VAL	B	919	-14.621	27.405	7.521	1.00	34.08
3179	CG2	VAL	B	919	-16.454	25.704	7.651	1.00	35.75
3180	N	LEU	B	920	-13.534	25.724	4.845	1.00	37.7
3181	CA	LEU	B	920	-13.721	25.873	3.409	1.00	38.54
3182	C	LEU	B	920	-13.611	24.497	2.741	1.00	39.82
3183	O	LEU	B	920	-14.03	24.315	1.595	1.00	39.67
3184	CB	LEU	B	920	-12.667	26.834	2.859	1.00	38.81
3185	CG	LEU	B	920	-12.887	27.515	1.509	1.00	38.99
3186	CD1	LEU	B	920	-14.273	28.126	1.433	1.00	40.07
3187	CD2	LEU	B	920	-11.831	28.588	1.333	1.00	38.69
3188	N	GLU	B	921	-13.057	23.53	3.471	1.00	40.58
3189	CA	GLU	B	921	-12.908	22.167	2.966	1.00	41.66
3190	C	GLU	B	921	-13.809	21.172	3.684	1.00	41.58
3191	O	GLU	B	921	-14.197	20.159	3.109	1.00	42.36
3192	CB	GLU	B	921	-11.469	21.689	3.103	1.00	43.43
3193	CG	GLU	B	921	-10.487	22.484	2.3	1.00	48.62
3194	CD	GLU	B	921	-9.125	21.842	2.273	1.00	51.68
3195	OE1	GLU	B	921	-8.566	21.6	3.363	1.00	54.25
3196	OE2	GLU	B	921	-8.616	21.577	1.162	1.00	54.42
3197	N	THR	B	922	-14.136	21.453	4.939	1.00	41.13

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TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

3198	CA	THR	B	922	-14.981	20.556	5.721	1.00	41.02
3199	C	THR	B	922	-16.466	20.905	5.655	1.00	41.41
3200	O	THR	B	922	-17.314	20.059	5.932	1.00	42.22
3201	CB	THR	B	922	-14.563	20.551	7.206	1.00	41.03
3202	OG1	THR	B	922	-14.671	21.881	7.736	1.00	41.04
3203	CG2	THR	B	922	-13.131	20.049	7.358	1.00	39.91
3204	N	ASP	B	923	-16.779	22.144	5.288	1.00	41.02
3205	CA	ASP	B	923	-18.168	22.595	5.209	1.00	40.33
3206	C	ASP	B	923	-18.23	23.932	4.474	1.00	39.66
3207	O	ASP	B	923	-18.56	24.96	5.064	1.00	38.58
3208	CB	ASP	B	923	-18.731	22.744	6.628	1.00	41.74
3209	CG	ASP	B	923	-20.186	23.179	6.645	1.00	42.59
3210	OD1	ASP	B	923	-20.809	23.255	5.562	1.00	44.02
3211	OD2	ASP	B	923	-20.709	23.442	7.75	1.00	42.55
3212	N	PRO	B	924	-17.917	23.929	3.164	1.00	39.41
3213	CA	PRO	B	924	-17.923	25.135	2.326	1.00	38.64
3214	C	PRO	B	924	-19.185	25.986	2.43	1.00	38.3
3215	O	PRO	B	924	-19.128	27.212	2.314	1.00	37.99
3216	CB	PRO	B	924	-17.687	24.584	0.918	1.00	38.42
3217	CG	PRO	B	924	-18.178	23.162	1.007	1.00	39.69
3218	CD	PRO	B	924	-17.671	22.728	2.347	1.00	38.72
3219	N	ALA	B	925	-20.321	25.338	2.651	1.00	38.52
3220	CA	ALA	B	925	-21.579	26.059	2.791	1.00	38.52
3221	C	ALA	B	925	-21.426	27.046	3.952	1.00	38.37
3222	O	ALA	B	925	-21.725	28.235	3.821	1.00	38.16
3223	CB	ALA	B	925	-22.716	25.076	3.066	1.00	37.65
3224	N	PHE	B	926	-20.944	26.54	5.084	1.00	38.6
3225	CA	PHE	B	926	-20.729	27.356	6.273	1.00	38.67
3226	C	PHE	B	926	-19.712	28.44	5.949	1.00	38.53
3227	O	PHE	B	926	-19.928	29.622	6.227	1.00	38.62
3228	CB	PHE	B	926	-20.185	26.492	7.416	1.00	40.29
3229	CG	PHE	B	926	-19.972	27.242	8.706	1.00	40.68
3230	CD1	PHE	B	926	-21.048	27.557	9.533	1.00	40.4
3231	CD2	PHE	B	926	-18.694	27.629	9.097	1.00	41.43
3232	CE1	PHE	B	926	-20.856	28.245	10.73	1.00	39.03
3233	CE2	PHE	B	926	-18.489	28.319	10.294	1.00	41.52
3234	CZ	PHE	B	926	-19.578	28.626	11.111	1.00	40.42
3235	N	ALA	B	927	-18.595	28.02	5.362	1.00	37.58
3236	CA	ALA	B	927	-17.525	28.938	5	1.00	36.68

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TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

3237	C	ALA	B	927	-18.036	30.11	4.176	1.00	36.64
3238	O	ALA	B	927	-17.769	31.267	4.501	1.00	36.35
3239	CB	ALA	B	927	-16.444	28.196	4.234	1.00	36.23
3240	N	ILE	B	928	-18.769	29.811	3.107	1.00	36.68
3241	CA	ILE	B	928	-19.298	30.858	2.239	1.00	37.4
3242	C	ILE	B	928	-20.311	31.728	2.968	1.00	37.58
3243	O	ILE	B	928	-20.293	32.957	2.845	1.00	37.39
3244	CB	ILE	B	928	-19.982	30.262	0.986	1.00	38.2
3245	CG1	ILE	B	928	-18.969	29.453	0.169	1.00	37.7
3246	CG2	ILE	B	928	-20.576	31.382	0.141	1.00	37.27
3247	CD1	ILE	B	928	-17.781	30.255	-0.291	1.00	37.71
3248	N	ALA	B	929	-21.192	31.084	3.727	1.00	37.95
3249	CA	ALA	B	929	-22.222	31.793	4.473	1.00	37.93
3250	C	ALA	B	929	-21.616	32.739	5.499	1.00	38.9
3251	O	ALA	B	929	-22.159	33.813	5.765	1.00	40.38
3252	CB	ALA	B	929	-23.138	30.796	5.164	1.00	37.11
3253	N	ASN	B	930	-20.483	32.349	6.071	1.00	38.61
3254	CA	ASN	B	930	-19.837	33.173	7.081	1.00	38.06
3255	C	ASN	B	930	-18.597	33.913	6.593	1.00	37.92
3256	O	ASN	B	930	-17.894	34.544	7.386	1.00	37.77
3257	CB	ASN	B	930	-19.51	32.309	8.295	1.00	38.46
3258	CG	ASN	B	930	-20.76	31.806	8.993	1.00	38.88
3259	OD1	ASN	B	930	-21.344	32.505	9.82	1.00	40.05
3260	ND2	ASN	B	930	-21.189	30.6	8.644	1.00	38
3261	N	SER	B	931	-18.34	33.844	5.287	1.00	35.72
3262	CA	SER	B	931	-17.197	34.53	4.687	1.00	34.65
3263	C	SER	B	931	-15.906	34.213	5.437	1.00	32.91
3264	O	SER	B	931	-15.043	35.08	5.604	1.00	32.93
3265	CB	SER	B	931	-17.422	36.048	4.715	1.00	35.04
3266	OG	SER	B	931	-18.753	36.382	4.362	1.00	37.36
3267	N	THR	B	932	-15.762	32.972	5.881	1.00	31.11
3268	CA	THR	B	932	-14.57	32.61	6.628	1.00	29.99
3269	C	THR	B	932	-13.861	31.368	6.112	1.00	28.11
3270	O	THR	B	932	-14.47	30.514	5.472	1.00	28.44
3271	CB	THR	B	932	-14.907	32.398	8.113	1.00	30.11
3272	OG1	THR	B	932	-13.694	32.327	8.868	1.00	31.62
3273	CG2	THR	B	932	-15.699	31.117	8.3	1.00	28.97
3274	N	ALA	B	933	-12.566	31.28	6.402	1.00	26.55
3275	CA	ALA	B	933	-11.749	30.147	5.987	1.00	25.56

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

3276	C	ALA	B	933	-11.444	29.245	7.179	1.00	24.55
3277	O	ALA	B	933	-10.832	28.186	7.031	1.00	23
3278	CB	ALA	B	933	-10.449	30.637	5.356	1.00	25.62
3279	N	SER	B	934	-11.877	29.665	8.363	1.00	24.13
3280	CA	SER	B	934	-11.633	28.878	9.566	1.00	25.77
3281	C	SER	B	934	-12.675	29.104	10.655	1.00	25.83
3282	O	SER	B	934	-13.294	30.165	10.737	1.00	25.44
3283	CB	SER	B	934	-10.24	29.199	10.135	1.00	24.87
3284	OG	SER	B	934	-9.953	28.379	11.26	1.00	24.16
3285	N	THR	B	935	-12.868	28.094	11.492	1.00	26.25
3286	CA	THR	B	935	-13.804	28.212	12.6	1.00	27.65
3287	C	THR	B	935	-13.098	28.996	13.701	1.00	28.33
3288	O	THR	B	935	-13.713	29.409	14.684	1.00	29.08
3289	CB	THR	B	935	-14.201	26.833	13.14	1.00	28.21
3290	OG1	THR	B	935	-13.022	26.038	13.332	1.00	28.42
3291	CG2	THR	B	935	-15.141	26.131	12.153	1.00	28.13
3292	N	LEU	B	936	-11.797	29.212	13.511	1.00	27.79
3293	CA	LEU	B	936	-10.977	29.93	14.479	1.00	27.81
3294	C	LEU	B	936	-10.666	31.357	14.028	1.00	27.35
3295	O	LEU	B	936	-10.376	31.605	12.858	1.00	27.91
3296	CB	LEU	B	936	-9.67	29.16	14.72	1.00	27.09
3297	CG	LEU	B	936	-9.793	27.699	15.192	1.00	27.29
3298	CD1	LEU	B	936	-8.433	27.004	15.104	1.00	25.69
3299	CD2	LEU	B	936	-10.331	27.663	16.619	1.00	26.33
3300	N	SER	B	937	-10.722	32.289	14.973	1.00	26.78
3301	CA	SER	B	937	-10.454	33.696	14.698	1.00	26.08
3302	C	SER	B	937	-8.972	34.017	14.874	1.00	25.9
3303	O	SER	B	937	-8.208	33.221	15.42	1.00	26.64
3304	CB	SER	B	937	-11.261	34.579	15.65	1.00	25.35
3305	OG	SER	B	937	-10.72	34.517	16.962	1.00	24.62
3306	N	SER	B	938	-8.575	35.191	14.405	1.00	26.48
3307	CA	SER	B	938	-7.196	35.632	14.526	1.00	27.34
3308	C	SER	B	938	-6.835	35.659	16.013	1.00	27.55
3309	O	SER	B	938	-5.764	35.195	16.41	1.00	27.28
3310	CB	SER	B	938	-7.037	37.024	13.908	1.00	27.07
3311	OG	SER	B	938	-5.704	37.489	14.028	1.00	28.03
3312	N	GLN	B	939	-7.739	36.191	16.831	1.00	27.2
3313	CA	GLN	B	939	-7.513	36.256	18.276	1.00	28.46
3314	C	GLN	B	939	-7.256	34.878	18.878	1.00	27.35

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

3315	O	GLN	B	939	-6.317	34.695	19.655	1.00	27.99
3316	CB	GLN	B	939	-8.713	36.896	18.983	1.00	29.16
3317	CG	GLN	B	939	-8.739	38.407	18.909	1.00	32.15
3318	CD	GLN	B	939	-7.632	39.046	19.73	1.00	32.99
3319	OE1	GLN	B	939	-6.78	39.757	19.199	1.00	33.6
3320	NE2	GLN	B	939	-7.643	38.794	21.033	1.00	32.9
3321	N	GLN	B	940	-8.103	33.915	18.532	1.00	26.11
3322	CA	GLN	B	940	-7.953	32.557	19.046	1.00	25.7
3323	C	GLN	B	940	-6.612	31.933	18.65	1.00	24.28
3324	O	GLN	B	940	-5.97	31.255	19.454	1.00	24.67
3325	CB	GLN	B	940	-9.103	31.679	18.546	1.00	26.1
3326	CG	GLN	B	940	-10.415	31.895	19.295	1.00	28.4
3327	CD	GLN	B	940	-11.595	31.182	18.641	1.00	31.2
3328	OE1	GLN	B	940	-12.484	30.67	19.327	1.00	32.16
3329	NE2	GLN	B	940	-11.614	31.162	17.309	1.00	29.85
3330	N	LEU	B	941	-6.194	32.167	17.411	1.00	23.07
3331	CA	LEU	B	941	-4.941	31.62	16.918	1.00	22.53
3332	C	LEU	B	941	-3.74	32.224	17.655	1.00	23.11
3333	O	LEU	B	941	-2.806	31.504	18.011	1.00	23.18
3334	CB	LEU	B	941	-4.835	31.848	15.408	1.00	22.05
3335	CG	LEU	B	941	-5.858	31.068	14.557	1.00	22.67
3336	CD1	LEU	B	941	-5.877	31.629	13.142	1.00	20.83
3337	CD2	LEU	B	941	-5.515	29.582	14.541	1.00	20.16
3338	N	LEU	B	942	-3.763	33.531	17.901	1.00	22.59
3339	CA	LEU	B	942	-2.657	34.165	18.619	1.00	23.45
3340	C	LEU	B	942	-2.625	33.714	20.079	1.00	22.78
3341	O	LEU	B	942	-1.558	33.635	20.682	1.00	21.09
3342	CB	LEU	B	942	-2.744	35.696	18.55	1.00	22.47
3343	CG	LEU	B	942	-2.446	36.372	17.206	1.00	23.78
3344	CD1	LEU	B	942	-2.403	37.884	17.417	1.00	25.27
3345	CD2	LEU	B	942	-1.124	35.9	16.629	1.00	23.95
3346	N	HIS	B	943	-3.792	33.422	20.645	1.00	23.41
3347	CA	HIS	B	943	-3.053	32.953	22.025	1.00	24.98
3348	C	HIS	B	943	-3.202	31.582	22.156	1.00	24.44
3349	O	HIS	B	943	-2.598	31.275	23.182	1.00	25.44
3350	CB	HIS	B	943	-5.298	32.896	22.516	1.00	27.58
3351	CG	HIS	B	943	-5.778	34.188	23.1	1.00	29.89
3352	ND1	HIS	B	943	-5.135	34.811	24.149	1.00	30.84
3353	CD2	HIS	B	943	-6.836	34.972	22.785	1.00	30.85

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

3354	CE1	HIS	B	943	-5.777	35.927	24.454	1.00	31.27
3355	NE2	HIS	B	943	-6.812	36.047	23.642	1.00	32.48
3356	N	PHE	B	944	-3.336	30.758	21.12	1.00	24.17
3357	CA	PHE	B	944	-2.706	29.438	21.107	1.00	23
3358	C	PHE	B	944	-1.196	29.695	21.126	1.00	22.12
3359	O	PHE	B	944	-0.457	29.08	21.896	1.00	20.95
3360	CB	PHE	B	944	-3.076	28.658	19.823	1.00	22.14
3361	CG	PHE	B	944	-4.427	27.967	19.875	1.00	22.11
3362	CD1	PHE	B	944	-5.203	27.846	18.723	1.00	22.84
3363	CD2	PHE	B	944	-4.918	27.439	21.066	1.00	22.41
3364	CE1	PHE	B	944	-6.446	27.211	18.752	1.00	23.28
3365	CE2	PHE	B	944	-6.164	26.798	21.115	1.00	22.57
3366	CZ	PHE	B	944	-6.931	26.689	19.955	1.00	24.56
3367	N	ALA	B	945	-0.748	30.619	20.276	1.00	20.49
3368	CA	ALA	B	945	0.677	30.942	20.19	1.00	20.08
3369	C	ALA	B	945	1.201	31.461	21.528	1.00	19.85
3370	O	ALA	B	945	2.276	31.06	21.976	1.00	18.42
3371	CB	ALA	B	945	0.926	31.979	19.077	1.00	18.47
3372	N	ALA	B	946	0.434	32.351	22.157	1.00	18.77
3373	CA	ALA	B	946	0.802	32.929	23.448	1.00	19.52
3374	C	ALA	B	946	0.833	31.842	24.528	1.00	19.76
3375	O	ALA	B	946	1.75	31.805	25.356	1.00	20.09
3376	CB	ALA	B	946	-0.186	34.034	23.833	1.00	18.89
3377	N	ASP	B	947	-0.176	30.972	24.522	1.00	19.66
3378	CA	ASP	B	947	-0.243	29.863	25.473	1.00	20.77
3379	C	ASP	B	947	1.041	29.024	25.437	1.00	20.3
3380	O	ASP	B	947	1.606	28.702	26.482	1.00	20.85
3381	CB	ASP	B	947	-1.43	28.943	25.152	1.00	22.18
3382	CG	ASP	B	947	-2.75	29.462	25.699	1.00	25.61
3383	OD1	ASP	B	947	-3.791	28.832	25.415	1.00	27.89
3384	OD2	ASP	B	947	-2.756	30.487	26.408	1.00	27.18
3385	N	VAL	B	948	1.493	28.66	24.237	1.00	18.23
3386	CA	VAL	B	948	2.709	27.854	24.109	1.00	19.29
3387	C	VAL	B	948	3.938	28.64	24.555	1.00	20.1
3388	O	VAL	B	948	4.845	28.081	25.167	1.00	20.19
3389	CB	VAL	B	948	2.943	27.359	22.636	1.00	17.88
3390	CG1	VAL	B	948	4.311	26.673	22.521	1.00	16.49
3391	CG2	VAL	B	948	1.847	26.379	22.227	1.00	16.39
3392	N	ALA	B	949	3.97	29.934	24.242	1.00	20.48

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

3393	CA	ALA	B	949	5.108	30.763	24.623	1.00	20.95
3394	C	ALA	B	949	5.158	30.897	26.143	1.00	20.01
3395	O	ALA	B	949	6.22	30.791	26.749	1.00	19.1
3396	CB	ALA	B	949	5.008	32.153	23.966	1.00	20.26
3397	N	ARG	B	950	4.001	31.137	26.75	1.00	20.72
3398	CA	ARG	B	950	3.914	31.268	28.201	1.00	21.55
3399	C	ARG	B	950	4.402	29.966	28.822	1.00	22.48
3400	O	ARG	B	950	5.205	29.972	29.756	1.00	22.54
3401	CB	ARG	B	950	2.46	31.528	28.628	1.00	21.69
3402	CG	ARG	B	950	2.275	31.782	30.125	1.00	21.25
3403	CD	ARG	B	950	0.804	32.046	30.485	1.00	22.98
3404	NE	ARG	B	950	0.189	33.018	29.583	1.00	23.53
3405	CZ	ARG	B	950	-0.677	32.711	28.618	1.00	25.52
3406	NH1	ARG	B	950	-1.056	31.448	28.418	1.00	23.47
3407	NH2	ARG	B	950	-1.145	33.667	27.831	1.00	23.47
3408	N	GLY	B	951	3.911	28.849	28.289	1.00	23.17
3409	CA	GLY	B	951	4.296	27.545	28.802	1.00	22.17
3410	C	GLY	B	951	5.769	27.236	28.62	1.00	22.6
3411	O	GLY	B	951	6.383	26.601	29.481	1.00	22.09
3412	N	MET	B	952	6.347	27.677	27.504	1.00	21.91
3413	CA	MET	B	952	7.758	27.416	27.256	1.00	23.25
3414	C	MET	B	952	8.653	28.316	28.094	1.00	23.02
3415	O	MET	B	952	9.778	27.948	28.423	1.00	22.68
3416	CB	MET	B	952	8.094	27.568	25.769	1.00	22.5
3417	CG	MET	B	952	7.73	26.337	24.93	1.00	22.92
3418	SD	MET	B	952	8.421	24.79	25.586	1.00	24.41
3419	CE	MET	B	952	10.174	25.049	25.278	1.00	22.84
3420	N	ASP	B	953	8.152	29.495	28.438	1.00	23.87
3421	CA	ASP	B	953	8.918	30.412	29.27	1.00	24.52
3422	C	ASP	B	953	9.034	29.728	30.63	1.00	24.75
3423	O	ASP	B	953	10.1	29.696	31.233	1.00	24.93
3424	CB	ASP	B	953	8.185	31.746	29.41	1.00	25.48
3425	CG	ASP	B	953	8.822	32.654	30.448	1.00	26.34
3426	OD1	ASP	B	953	8.106	33.081	31.375	1.00	27.98
3427	OD2	ASP	B	953	10.03	32.941	30.34	1.00	25.54
3428	N	TYR	B	954	7.925	29.161	31.094	1.00	24.24
3429	CA	TYR	B	954	7.896	28.449	32.364	1.00	23.77
3430	C	TYR	B	954	8.881	27.264	32.391	1.00	24.57
3431	O	TYR	B	954	9.63	27.091	33.354	1.00	24.42

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TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

3432	CB	TYR	B	954	6.483	27.936	32.636	1.00	24.09
3433	CG	TYR	B	954	6.392	26.989	33.811	1.00	24.89
3434	CD1	TYR	B	954	6.278	27.467	35.12	1.00	26.28
3435	CD2	TYR	B	954	6.441	25.61	33.614	1.00	26.23
3436	CE1	TYR	B	954	6.214	26.583	36.207	1.00	26.48
3437	CE2	TYR	B	954	6.375	24.722	34.682	1.00	27.42
3438	CZ	TYR	B	954	6.262	25.212	35.975	1.00	27.76
3439	OH	TYR	B	954	6.192	24.323	37.018	1.00	27.08
3440	N	LEU	B	955	8.866	26.444	31.342	1.00	23.69
3441	CA	LEU	B	955	9.75	25.282	31.264	1.00	24.31
3442	C	LEU	B	955	11.211	25.678	31.038	1.00	25.62
3443	O	LEU	B	955	12.129	25.11	31.636	1.00	26.15
3444	CB	LEU	B	955	9.289	24.347	30.137	1.00	23.14
3445	CG	LEU	B	955	7.97	23.599	30.368	1.00	22.6
3446	CD1	LEU	B	955	7.605	22.785	29.136	1.00	21.81
3447	CD2	LEU	B	955	8.114	22.687	31.575	1.00	21.65
3448	N	SER	B	956	11.41	26.656	30.165	1.00	26.86
3449	CA	SER	B	956	12.733	27.154	29.833	1.00	28.34
3450	C	SER	B	956	13.438	27.674	31.085	1.00	28.97
3451	O	SER	B	956	14.61	27.379	31.317	1.00	27.9
3452	CB	SER	B	956	12.606	28.283	28.805	1.00	29.86
3453	OG	SER	B	956	13.873	28.812	28.466	1.00	35.29
3454	N	GLN	B	957	12.713	28.449	31.887	1.00	29.79
3455	CA	GLN	B	957	13.273	29.013	33.109	1.00	31.45
3456	C	GLN	B	957	13.596	27.954	34.156	1.00	31.19
3457	O	GLN	B	957	14.212	28.252	35.171	1.00	30.95
3458	CB	GLN	B	957	12.332	30.074	33.697	1.00	33.69
3459	CG	GLN	B	957	12.44	31.424	32.993	1.00	38.67
3460	CD	GLN	B	957	11.854	32.569	33.808	1.00	41.63
3461	OE1	GLN	B	957	12.108	32.681	35.011	1.00	43.91
3462	NE2	GLN	B	957	11.084	33.437	33.151	1.00	42.36
3463	N	LYS	B	958	13.19	26.716	33.905	1.00	30.94
3464	CA	LYS	B	958	13.483	25.635	34.831	1.00	30.9
3465	C	LYS	B	958	14.474	24.662	34.204	1.00	30.44
3466	O	LYS	B	958	14.553	23.501	34.599	1.00	31.21
3467	CB	LYS	B	958	12.201	24.907	35.226	1.00	32.53
3468	CG	LYS	B	958	11.171	25.819	35.874	1.00	35.41
3469	CD	LYS	B	958	10.952	25.49	37.333	1.00	37.72
3470	CE	LYS	B	958	10.231	24.168	37.481	1.00	39.12



TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

3471	NZ	LYS	B	958	8.987	24.187	36.676	1.00	40.92
3472	N	GLN	B	959	15.213	25.144	33.21	1.00	30.46
3473	CA	GLN	B	959	16.239	24.355	32.524	1.00	30.41
3474	C	GLN	B	959	15.756	23.295	31.536	1.00	28.36
3475	O	GLN	B	959	16.567	22.538	31.011	1.00	28.14
3476	CB	GLN	B	959	17.162	23.683	33.552	1.00	34.79
3477	CG	GLN	B	959	17.792	24.636	34.567	1.00	40.16
3478	CD	GLN	B	959	18.665	25.692	33.915	1.00	44.35
3479	OE1	GLN	B	959	19.697	25.38	33.307	1.00	46.41
3480	NE2	GLN	B	959	18.256	26.955	34.035	1.00	45.72
3481	N	PHE	B	960	14.456	23.217	31.28	1.00	26.8
3482	CA	PHE	B	960	13.972	22.217	30.329	1.00	25.06
3483	C	PHE	B	960	14.283	22.596	28.889	1.00	23.28
3484	O	PHE	B	960	14.22	23.769	28.514	1.00	23.5
3485	CB	PHE	B	960	12.461	22.012	30.437	1.00	25.51
3486	CG	PHE	B	960	12.037	21.221	31.628	1.00	26.88
3487	CD1	PHE	B	960	11.868	21.834	32.864	1.00	27.38
3488	CD2	PHE	B	960	11.781	19.858	31.512	1.00	27.49
3489	CE1	PHE	B	960	11.453	21.099	33.965	1.00	28.27
3490	CE2	PHE	B	960	11.365	19.115	32.605	1.00	27.24
3491	CZ	PHE	B	960	11.198	19.734	33.835	1.00	28.68
3492	N	ILE	B	961	14.623	21.583	28.102	1.00	21.74
3493	CA	ILE	B	961	14.902	21.717	26.678	1.00	20.99
3494	C	ILE	B	961	13.947	20.695	26.056	1.00	21.5
3495	O	ILE	B	961	14.056	19.496	26.318	1.00	21.02
3496	CB	ILE	B	961	16.369	21.351	26.337	1.00	20.11
3497	CG1	ILE	B	961	17.33	22.233	27.143	1.00	19.94
3498	CG2	ILE	B	961	16.627	21.559	24.846	1.00	18.73
3499	CD1	ILE	B	961	18.822	21.93	26.912	1.00	18.39
3500	N	HIS	B	962	12.994	21.179	25.263	1.00	21.93
3501	CA	HIS	B	962	11.986	20.325	24.634	1.00	22.6
3502	C	HIS	B	962	12.519	19.393	23.546	1.00	23.35
3503	O	HIS	B	962	12.253	18.195	23.577	1.00	22.84
3504	CB	HIS	B	962	10.853	21.196	24.067	1.00	23
3505	CG	HIS	B	962	9.591	20.44	23.8	1.00	22.21
3506	ND1	HIS	B	962	9.436	19.607	22.711	1.00	20.85
3507	CD2	HIS	B	962	8.449	20.331	24.523	1.00	21.95
3508	CE1	HIS	B	962	8.258	19.014	22.779	1.00	21.33
3509	NE2	HIS	B	962	7.639	19.434	23.868	1.00	22.54

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TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

3510	N	ARG	B	963	13.254	19.95	22.585	1.00	24.29
3511	CA	ARG	B	963	13.85	19.195	21.473	1.00	25.83
3512	C	ARG	B	963	12.909	18.889	20.303	1.00	26.63
3513	O	ARG	B	963	13.371	18.602	19.197	1.00	25.86
3514	CB	ARG	B	963	14.443	17.857	21.946	1.00	26.4
3515	CG	ARG	B	963	15.522	17.922	23.024	1.00	28.03
3516	CD	ARG	B	963	16.271	16.581	23.092	1.00	27.78
3517	NE	ARG	B	963	15.359	15.447	22.932	1.00	29.76
3518	CZ	ARG	B	963	14.535	14.989	23.873	1.00	31.22
3519	NH1	ARG	B	963	14.494	15.55	25.075	1.00	32
3520	NH2	ARG	B	963	13.725	13.975	23.604	1.00	31.75
3521	N	ASP	B	964	11.601	18.938	20.531	1.00	26.57
3522	CA	ASP	B	964	10.662	18.627	19.457	1.00	27.22
3523	C	ASP	B	964	9.38	19.462	19.536	1.00	26.18
3524	O	ASP	B	964	8.266	18.933	19.542	1.00	25.63
3525	CB	ASP	B	964	10.346	17.124	19.492	1.00	29.56
3526	CG	ASP	B	964	9.491	16.674	18.32	1.00	32.5
3527	OD1	ASP	B	964	9.672	17.198	17.203	1.00	32.35
3528	OD2	ASP	B	964	8.643	15.783	18.521	1.00	35.21
3529	N	LEU	B	965	9.558	20.775	19.586	1.00	24.81
3530	CA	LEU	B	965	8.444	21.708	19.675	1.00	25.25
3531	C	LEU	B	965	7.759	21.845	18.318	1.00	24.56
3532	O	LEU	B	965	8.367	22.297	17.349	1.00	27.11
3533	CB	LEU	B	965	8.967	23.064	20.142	1.00	26.04
3534	CG	LEU	B	965	8.059	23.977	20.962	1.00	28.42
3535	CD1	LEU	B	965	7.395	23.194	22.113	1.00	26.98
3536	CD2	LEU	B	965	8.909	25.137	21.502	1.00	25.78
3537	N	ALA	B	966	6.494	21.45	18.255	1.00	22.81
3538	CA	ALA	B	966	5.72	21.513	17.021	1.00	21.42
3539	C	ALA	B	966	4.256	21.336	17.387	1.00	20.97
3540	O	ALA	B	966	3.944	20.837	18.473	1.00	19.85
3541	CB	ALA	B	966	6.159	20.404	16.062	1.00	20.48
3542	N	ALA	B	967	3.367	21.735	16.48	1.00	19
3543	CA	ALA	B	967	1.933	21.634	16.722	1.00	19.2
3544	C	ALA	B	967	1.46	20.23	17.101	1.00	19.46
3545	O	ALA	B	967	0.508	20.083	17.871	1.00	19.23
3546	CB	ALA	B	967	1.167	22.127	15.505	1.00	18.58
3547	N	ARG	B	968	2.108	19.201	16.557	1.00	19.39
3548	CA	ARG	B	968	1.725	17.829	16.884	1.00	20.51

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

3549	C	ARG	B	968	1.993	17.556	18.363	1.00	19.62
3550	O	ARG	B	968	1.367	16.681	18.957	1.00	18.84
3551	CB	ARG	B	968	2.51	16.816	16.032	1.00	21.59
3552	CG	ARG	B	968	4.014	16.933	16.193	1.00	22.29
3553	CD	ARG	B	968	4.787	15.853	15.447	1.00	23.33
3554	NE	ARG	B	968	6.216	16.158	15.457	1.00	23.56
3555	CZ	ARG	B	968	6.799	16.999	14.609	1.00	26.5
3556	NH1	ARG	B	968	6.074	17.604	13.679	1.00	28.03
3557	NH2	ARG	B	968	8.096	17.262	14.703	1.00	25.53
3558	N	ASN	B	969	2.928	18.297	18.956	1.00	19.91
3559	CA	ASN	B	969	3.245	18.099	20.369	1.00	20.67
3560	C	ASN	B	969	2.576	19.087	21.316	1.00	20.77
3561	O	ASN	B	969	2.998	19.244	22.469	1.00	21.73
3562	CB	ASN	B	969	4.762	18.095	20.597	1.00	21.16
3563	CG	ASN	B	969	5.397	16.754	20.245	1.00	21.91
3564	OD1	ASN	B	969	4.824	15.702	20.516	1.00	22.99
3565	ND2	ASN	B	969	6.591	16.788	19.659	1.00	21.1
3566	N	ILE	B	970	1.532	19.751	20.83	1.00	20.17
3567	CA	ILE	B	970	0.776	20.69	21.65	1.00	19.79
3568	C	ILE	B	970	-0.644	20.132	21.707	1.00	21.54
3569	O	ILE	B	970	-1.205	19.745	20.676	1.00	21.83
3570	CB	ILE	B	970	0.722	22.098	21.025	1.00	19.2
3571	CG1	ILE	B	970	2.137	22.658	20.857	1.00	19.95
3572	CG2	ILE	B	970	-0.142	23.019	21.893	1.00	17.6
3573	CD1	ILE	B	970	2.927	22.835	22.161	1.00	17.14
3574	N	LEU	B	971	-1.216	20.065	22.904	1.00	20.48
3575	CA	LEU	B	971	-2.571	19.56	23.061	1.00	20.72
3576	C	LEU	B	971	-3.539	20.709	23.332	1.00	20.82
3577	O	LEU	B	971	-3.187	21.696	23.987	1.00	19.84
3578	CB	LEU	B	971	-2.64	18.539	24.212	1.00	19.53
3579	CG	LEU	B	971	-1.94	17.171	24.105	1.00	19.56
3580	CD1	LEU	B	971	-2.433	16.442	22.859	1.00	19.87
3581	CD2	LEU	B	971	-0.428	17.338	24.046	1.00	20.36
3582	N	VAL	B	972	-4.752	20.588	22.801	1.00	22.47
3583	CA	VAL	B	972	-5.792	21.591	23	1.00	23.2
3584	C	VAL	B	972	-6.643	21.053	24.142	1.00	25.64
3585	O	VAL	B	972	-7.509	20.19	23.947	1.00	24.11
3586	CB	VAL	B	972	-6.659	21.768	21.732	1.00	23.99
3587	CG1	VAL	B	972	-7.779	22.788	21.99	1.00	22.81

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

3588	CG2	VAL	B	972	-5.779	22.235	20.568	1.00	23.98
3589	N	GLY	B	973	-6.383	21.564	25.34	1.00	26.74
3590	CA	GLY	B	973	-7.098	21.09	26.508	1.00	29.59
3591	C	GLY	B	973	-8.458	21.691	26.764	1.00	31.17
3592	O	GLY	B	973	-9.054	22.338	25.905	1.00	29.29
3593	N	GLU	B	974	-8.947	21.453	27.975	1.00	35.4
3594	CA	GLU	B	974	-10.238	21.955	28.415	1.00	38.05
3595	C	GLU	B	974	-10.266	23.472	28.239	1.00	37.86
3596	O	GLU	B	974	-9.261	24.153	28.468	1.00	37.5
3597	CB	GLU	B	974	-10.453	21.585	29.887	1.00	41.73
3598	CG	GLU	B	974	-11.851	21.875	30.416	1.00	47.56
3599	CD	GLU	B	974	-12.925	21.078	29.696	1.00	49.87
3600	OE1	GLU	B	974	-12.803	19.834	29.646	1.00	52.49
3601	OE2	GLU	B	974	-13.888	21.692	29.185	1.00	51.7
3602	N	ASN	B	975	-11.416	23.992	27.819	1.00	37.65
3603	CA	ASN	B	975	-11.584	25.422	27.605	1.00	37.4
3604	C	ASN	B	975	-10.696	25.905	26.464	1.00	35.2
3605	O	ASN	B	975	-10.479	27.101	26.296	1.00	34.36
3606	CB	ASN	B	975	-11.255	26.178	28.895	1.00	41.39
3607	CG	ASN	B	975	-12.248	25.885	30.009	1.00	46.17
3608	OD1	ASN	B	975	-11.975	26.138	31.186	1.00	49.16
3609	ND2	ASN	B	975	-13.412	25.355	29.642	1.00	47.95
3610	N	TYR	B	976	-10.195	24.956	25.68	1.00	33.32
3611	CA	TYR	B	976	-9.323	25.239	24.545	1.00	31.94
3612	C	TYR	B	976	-7.986	25.874	24.926	1.00	30.81
3613	O	TYR	B	976	-7.441	26.693	24.188	1.00	31.83
3614	CB	TYR	B	976	-10.049	26.112	23.518	1.00	33.46
3615	CG	TYR	B	976	-11.329	25.483	23.011	1.00	36.7
3616	CD1	TYR	B	976	-12.553	25.731	23.641	1.00	37.61
3617	CD2	TYR	B	976	-11.312	24.593	21.933	1.00	37.59
3618	CE1	TYR	B	976	-13.726	25.107	23.214	1.00	37.66
3619	CE2	TYR	B	976	-12.476	23.966	21.498	1.00	38.07
3620	CZ	TYR	B	976	-13.679	24.226	22.144	1.00	39.26
3621	OH	TYR	B	976	-14.828	23.593	21.724	1.00	40.39
3622	N	VAL	B	977	-7.464	25.491	26.086	1.00	28.76
3623	CA	VAL	B	977	-6.174	25.988	26.561	1.00	27.72
3624	C	VAL	B	977	-5.063	25.104	25.979	1.00	26.34
3625	O	VAL	B	977	-5.077	23.889	26.154	1.00	26.64
3626	CB	VAL	B	977	-6.09	25.936	28.106	1.00	27.9

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

3627	CG1	VAL	B	977	-4.695	26.339	28.574	1.00	27.85
3628	CG2	VAL	B	977	-7.144	26.855	28.714	1.00	27.46
3629	N	ALA	B	978	-4.105	25.706	25.285	1.00	25.08
3630	CA	ALA	B	978	-3.011	24.938	24.698	1.00	23.75
3631	C	ALA	B	978	-2.04	24.465	25.777	1.00	23.69
3632	O	ALA	B	978	-1.566	25.266	26.592	1.00	22.92
3633	CB	ALA	B	978	-2.279	25.775	23.665	1.00	22.33
3634	N	LYS	B	979	-1.761	23.16	25.778	1.00	23.44
3635	CA	LYS	B	979	-0.852	22.545	26.745	1.00	23.14
3636	C	LYS	B	979	0.306	21.827	26.063	1.00	22.77
3637	O	LYS	B	979	0.098	21.004	25.171	1.00	23.09
3638	CB	LYS	B	979	-1.611	21.556	27.626	1.00	22.92
3639	CG	LYS	B	979	-2.589	22.22	28.587	1.00	25.4
3640	CD	LYS	B	979	-3.425	21.205	29.348	1.00	25.08
3641	CE	LYS	B	979	-4.247	21.878	30.434	1.00	27.52
3642	NZ	LYS	B	979	-3.361	22.399	31.516	1.00	28.64
3643	N	ILE	B	980	1.528	22.142	26.487	1.00	21.54
3644	CA	ILE	B	980	2.716	21.523	25.914	1.00	21.03
3645	C	ILE	B	980	2.879	20.065	26.376	1.00	20.98
3646	O	ILE	B	980	2.813	19.781	27.579	1.00	19.75
3647	CB	ILE	B	980	3.986	22.327	26.304	1.00	21.14
3648	CG1	ILE	B	980	3.87	23.762	25.789	1.00	21.63
3649	CG2	ILE	B	980	5.236	21.679	25.716	1.00	18.58
3650	CD1	ILE	B	980	4.953	24.7	26.317	1.00	20.2
3651	N	ALA	B	981	3.069	19.15	25.42	1.00	21.3
3652	CA	ALA	B	981	3.286	17.728	25.726	1.00	22.19
3653	C	ALA	B	981	4.695	17.697	26.296	1.00	22.62
3654	O	ALA	B	981	5.644	18.137	25.64	1.00	22.01
3655	CB	ALA	B	981	3.21	16.879	24.458	1.00	21.93
3656	N	ASP	B	982	4.832	17.157	27.501	1.00	23.09
3657	CA	ASP	B	982	6.115	17.167	28.187	1.00	24.63
3658	C	ASP	B	982	6.723	15.846	28.65	1.00	25.76
3659	O	ASP	B	982	7.28	15.777	29.748	1.00	26.66
3660	CB	ASP	B	982	6.006	18.123	29.381	1.00	23.68
3661	CG	ASP	B	982	4.729	17.905	30.194	1.00	23.19
3662	OD1	ASP	B	982	4.386	18.781	31.018	1.00	23.73
3663	OD2	ASP	B	982	4.066	16.863	30.017	1.00	22.28
3664	N	PHE	B	983	6.637	14.812	27.819	1.00	25.6
3665	CA	PHE	B	983	7.21	13.519	28.168	1.00	26.4

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

3666	C	PHE	B	983	8.572	13.357	27.488	1.00	27.35
3667	O	PHE	B	983	8.739	13.721	26.324	1.00	26.9
3668	CB	PHE	B	983	6.288	12.376	27.73	1.00	26.21
3669	CG	PHE	B	983	6.771	11.014	28.156	1.00	26.44
3670	CD1	PHE	B	983	6.516	10.539	29.44	1.00	26.08
3671	CD2	PHE	B	983	7.53	10.227	27.291	1.00	26.23
3672	CE1	PHE	B	983	7.014	9.304	29.856	1.00	25.48
3673	CE2	PHE	B	983	8.031	8.993	27.7	1.00	25.14
3674	CZ	PHE	B	983	7.773	8.532	28.984	1.00	24.29
3675	N	GLY	B	984	9.543	12.819	28.222	1.00	27.38
3676	CA	GLY	B	984	10.869	12.612	27.663	1.00	27.36
3677	C	GLY	B	984	11.672	13.862	27.344	1.00	27.41
3678	O	GLY	B	984	12.509	13.847	26.441	1.00	28.38
3679	N	LEU	B	985	11.437	14.951	28.066	1.00	26.59
3680	CA	LEU	B	985	12.186	16.174	27.799	1.00	26.69
3681	C	LEU	B	985	13.566	16.115	28.447	1.00	26.92
3682	O	LEU	B	985	13.817	15.294	29.333	1.00	25.89
3683	CB	LEU	B	985	11.434	17.399	28.331	1.00	25.81
3684	CG	LEU	B	985	9.989	17.594	27.854	1.00	26.26
3685	CD1	LEU	B	985	9.53	18.98	28.279	1.00	24.43
3686	CD2	LEU	B	985	9.889	17.435	26.33	1.00	24.1
3687	N	SER	B	986	14.459	16.985	27.989	1.00	26.44
3688	CA	SER	B	986	15.803	17.051	28.534	1.00	25.92
3689	C	SER	B	986	15.875	18.214	29.508	1.00	25.97
3690	O	SER	B	986	15.032	19.111	29.497	1.00	23.63
3691	CB	SER	B	986	16.834	17.237	27.422	1.00	26.46
3692	OG	SER	B	986	16.886	16.091	26.589	1.00	27.79
3693	N	ARG	B	987	16.895	18.195	30.351	1.00	26.25
3694	CA	ARG	B	987	17.055	19.232	31.344	1.00	27.64
3695	C	ARG	B	987	18.528	19.575	31.492	1.00	27.49
3696	O	ARG	B	987	19.35	18.687	31.689	1.00	27.95
3697	CB	ARG	B	987	16.484	18.73	32.663	1.00	28.84
3698	CG	ARG	B	987	16.185	19.815	33.646	1.00	32.35
3699	CD	ARG	B	987	14.986	19.447	34.486	1.00	34.37
3700	NE	ARG	B	987	14.728	20.493	35.46	1.00	37.59
3701	CZ	ARG	B	987	15.515	20.74	36.497	1.00	39.02
3702	NH1	ARG	B	987	16.602	20.004	36.692	1.00	39.53
3703	NH2	ARG	B	987	15.226	21.735	37.324	1.00	40.03
3704	N	GLY	B	988	18.855	20.86	31.391	1.00	27.3

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

3705	CA	GLY	B	988	20.24	21.282	31.509	1.00	28.11
3706	C	GLY	B	988	20.637	22.422	30.58	1.00	29.29
3707	O	GLY	B	988	19.793	23.142	30.053	1.00	29.48
3708	N	GLN	B	989	21.94	22.577	30.384	1.00	29.7
3709	CA	GLN	B	989	22.506	23.624	29.537	1.00	31.39
3710	C	GLN	B	989	22.325	23.362	28.039	1.00	31.27
3711	O	GLN	B	989	21.83	24.21	27.292	1.00	30.41
3712	CB	GLN	B	989	24	23.746	29.86	1.00	34
3713	CG	GLN	B	989	24.836	24.548	28.877	1.00	37.62
3714	CD	GLN	B	989	24.93	26.005	29.247	1.00	40.96
3715	OE1	GLN	B	989	25.985	26.626	29.105	1.00	42.48
3716	NE2	GLN	B	989	23.825	26.568	29.72	1.00	42.79
3717	N	GLU	B	990	22.741	22.176	27.612	1.00	30.96
3718	CA	GLU	B	990	22.663	21.775	26.213	1.00	30.65
3719	C	GLU	B	990	22.649	20.258	26.152	1.00	30.38
3720	O	GLU	B	990	23.29	19.593	26.968	1.00	30.13
3721	CB	GLU	B	990	23.871	22.326	25.447	1.00	29.99
3722	CG	GLU	B	990	24.11	21.701	24.088	1.00	33.25
3723	CD	GLU	B	990	25.206	22.413	23.307	1.00	34.81
3724	OE1	GLU	B	990	24.91	23.421	22.637	1.00	35.49
3725	OE2	GLU	B	990	26.371	21.974	23.37	1.00	37.41
3726	N	VAL	B	991	21.905	19.703	25.204	1.00	28.88
3727	CA	VAL	B	991	21.854	18.26	25.087	1.00	28.9
3728	C	VAL	B	991	22.165	17.79	23.675	1.00	29.45
3729	O	VAL	B	991	21.683	18.351	22.69	1.00	30.08
3730	CB	VAL	B	991	20.485	17.703	25.53	1.00	28.33
3731	CG1	VAL	B	991	19.383	18.236	24.639	1.00	28.58
3732	CG2	VAL	B	991	20.515	16.185	25.5	1.00	29.41
3733	N	TYR	B	992	22.999	16.766	23.591	1.00	29.35
3734	CA	TYR	B	992	23.379	16.186	22.314	1.00	30.81
3735	C	TYR	B	992	22.612	14.874	22.132	1.00	31.32
3736	O	TYR	B	992	22.641	14.005	23.012	1.00	30.56
3737	CB	TYR	B	992	24.88	15.913	22.291	1.00	30.06
3738	CG	TYR	B	992	25.3	14.946	21.212	1.00	31.34
3739	CD1	TYR	B	992	25.555	15.382	19.911	1.00	30.39
3740	CD2	TYR	B	992	25.406	13.586	21.486	1.00	31.5
3741	CE1	TYR	B	992	25.905	14.477	18.912	1.00	32.06
3742	CE2	TYR	B	992	25.751	12.678	20.501	1.00	32.79
3743	CZ	TYR	B	992	26	13.124	19.221	1.00	32.4

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

3744	OH	TYR	B	992	26.348	12.206	18.266	1.00	33.91
3745	N	VAL	B	993	21.916	14.745	21.001	1.00	31.86
3746	CA	VAL	B	993	21.154	13.533	20.692	1.00	34.05
3747	C	VAL	B	993	21.496	13.08	19.27	1.00	36.09
3748	O	VAL	B	993	21.134	13.739	18.294	1.00	35.11
3749	CB	VAL	B	993	19.638	13.772	20.809	1.00	33.42
3750	CG1	VAL	B	993	18.896	12.46	20.62	1.00	33.48
3751	CG2	VAL	B	993	19.306	14.368	22.169	1.00	32.13
3752	N	ALA	B	994	22.193	11.948	19.171	1.00	39.05
3753	CA	ALA	B	994	22.646	11.391	17.892	1.00	42.54
3754	C	ALA	B	994	21.613	11.206	16.776	1.00	44.74
3755	O	ALA	B	994	21.779	11.774	15.694	1.00	45.67
3756	CB	ALA	B	994	23.378	10.065	18.141	1.00	41.75
3757	N	ALA	B	995	20.576	10.409	17.038	1.00	47.28
3758	CA	ALA	B	995	19.507	10.102	16.071	1.00	49.7
3759	C	ALA	B	995	19.505	8.602	15.775	1.00	50.63
3760	OT1	ALA	B	995	20.333	8.182	14.933	1.00	51.45
3761	CB	ALA	B	995	19.682	10.882	14.747	1.00	49.14
3762	OT2	ALA	B	995	18.702	7.868	16.398	1.00	51.42
3763	N	ALA	B	0	12.307	9.575	10.93	1.00	58.65
3764	CA	ALA	B	0	12.332	9.501	12.42	1.00	58.2
3765	C	ALA	B	0	12.989	10.74	13.022	1.00	57.07
3766	O	ALA	B	0	13.325	10.76	14.206	1.00	58.18
3767	CB	ALA	B	0	13.08	8.243	12.868	1.00	59.16
3768	N	LEU	B	1	13.165	11.773	12.204	1.00	55.09
3769	CA	LEU	B	1	13.789	13.013	12.659	1.00	52.41
3770	C	LEU	B	1	12.994	14.234	12.161	1.00	49.61
3771	O	LEU	B	1	12.802	14.407	10.956	1.00	50.28
3772	CB	LEU	B	1	15.235	13.066	12.15	1.00	52.84
3773	CG	LEU	B	1	16.26	13.846	12.981	1.00	53.21
3774	CD1	LEU	B	1	16.393	13.222	14.37	1.00	52.55
3775	CD2	LEU	B	1	17.6	13.833	12.264	1.00	52.92
3776	N	PRO	B	2	12.524	15.096	13.088	1.00	46.44
3777	CA	PRO	B	2	11.745	16.303	12.776	1.00	42.51
3778	C	PRO	B	2	12.586	17.414	12.139	1.00	39.16
3779	O	PRO	B	2	12.656	18.537	12.644	1.00	37.84
3780	CB	PRO	B	2	11.195	16.704	14.136	1.00	43.24
3781	CG	PRO	B	2	12.347	16.359	15.047	1.00	44.06
3782	CD	PRO	B	2	12.757	14.989	14.542	1.00	45.51



TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

3783	N	VAL	B	3	13.21	17.085	11.017	1.00	35.57
3784	CA	VAL	B	3	14.066	18.009	10.286	1.00	32.79
3785	C	VAL	B	3	13.493	19.407	10.041	1.00	30.21
3786	O	VAL	B	3	14.203	20.403	10.18	1.00	29.24
3787	CB	VAL	B	3	14.451	17.41	8.913	1.00	33.63
3788	CG1	VAL	B	3	15.366	18.373	8.158	1.00	33.18
3789	CG2	VAL	B	3	15.121	16.056	9.109	1.00	33.3
3790	N	ARG	B	4	12.218	19.474	9.671	1.00	28.1
3791	CA	ARG	B	4	11.564	20.741	9.36	1.00	26.86
3792	C	ARG	B	4	11.386	21.713	10.529	1.00	25.86
3793	O	ARG	B	4	11.062	22.878	10.314	1.00	24.8
3794	CB	ARG	B	4	10.209	20.463	8.694	1.00	28.47
3795	CG	ARG	B	4	10.329	19.692	7.389	1.00	29.76
3796	CD	ARG	B	4	9.032	18.993	6.996	1.00	30.46
3797	NE	ARG	B	4	9.283	18.037	5.923	1.00	29.41
3798	CZ	ARG	B	4	9.453	18.356	4.64	1.00	31.6
3799	NH1	ARG	B	4	9.393	19.622	4.239	1.00	29.6
3800	NH2	ARG	B	4	9.709	17.402	3.749	1.00	32.31
3801	N	TRP	B	5	11.602	21.239	11.754	1.00	24.39
3802	CA	TRP	B	5	11.469	22.078	12.946	1.00	25.65
3803	C	TRP	B	5	12.822	22.313	13.624	1.00	26.1
3804	O	TRP	B	5	12.932	23.09	14.573	1.00	26.79
3805	CB	TRP	B	5	10.521	21.414	13.947	1.00	24.76
3806	CG	TRP	B	5	9.076	21.517	13.592	1.00	25.18
3807	CD1	TRP	B	5	8.174	22.427	14.075	1.00	25.07
3808	CD2	TRP	B	5	8.355	20.689	12.675	1.00	23.55
3809	NE1	TRP	B	5	6.939	22.212	13.517	1.00	24
3810	CE2	TRP	B	5	7.02	21.151	12.649	1.00	24.79
3811	CE3	TRP	B	5	8.707	19.597	11.862	1.00	24.85
3812	CZ2	TRP	B	5	6.026	20.558	11.849	1.00	23.9
3813	CZ3	TRP	B	5	7.718	19.003	11.064	1.00	24.26
3814	CH2	TRP	B	5	6.398	19.49	11.064	1.00	24.17
3815	N	MET	B	6	13.851	21.64	13.122	1.00	26.22
3816	CA	MET	B	6	15.185	21.734	13.69	1.00	26.28
3817	C	MET	B	6	15.985	22.97	13.322	1.00	26.34
3818	O	MET	B	6	16.014	23.396	12.174	1.00	25.72
3819	CB	MET	B	6	15.981	20.474	13.329	1.00	28.16
3820	CG	MET	B	6	15.504	19.236	14.074	1.00	28.53
3821	SD	MET	B	6	16.201	17.702	13.473	1.00	31.25

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

3822	CE	MET	B	6	17.977	18.005	13.71	1.00	28.53
3823	N	ALA	B	7	16.644	23.539	14.325	1.00	26.69
3824	CA	ALA	B	7	17.471	24.72	14.136	1.00	26.81
3825	C	ALA	B	7	18.76	24.332	13.408	1.00	27.1
3826	O	ALA	B	7	19.182	23.178	13.446	1.00	26.68
3827	CB	ALA	B	7	17.799	25.344	15.497	1.00	26.03
3828	N	ILE	B	8	19.382	25.307	12.756	1.00	27.61
3829	CA	ILE	B	8	20.615	25.075	12.023	1.00	28.95
3830	C	ILE	B	8	21.662	24.318	12.832	1.00	28.72
3831	O	ILE	B	8	22.256	23.362	12.327	1.00	28.82
3832	CB	ILE	B	8	21.221	26.405	11.527	1.00	31.3
3833	CG1	ILE	B	8	20.373	26.948	10.37	1.00	32.08
3834	CG2	ILE	B	8	22.667	26.196	11.083	1.00	31.61
3835	CD1	ILE	B	8	20.755	28.353	9.929	1.00	34.51
3836	N	GLU	B	9	21.889	24.732	14.079	1.00	28.17
3837	CA	GLU	B	9	22.887	24.055	14.91	1.00	28.18
3838	C	GLU	B	9	22.501	22.602	15.197	1.00	27.92
3839	O	GLU	B	9	23.371	21.746	15.364	1.00	28.05
3840	CB	GLU	B	9	23.118	24.808	16.232	1.00	27.12
3841	CG	GLU	B	9	21.907	24.898	17.136	1.00	26.26
3842	CD	GLU	B	9	21.106	26.172	16.928	1.00	26.69
3843	OE1	GLU	B	9	21.112	26.705	15.796	1.00	25.75
3844	OE2	GLU	B	9	20.461	26.63	17.898	1.00	26.34
3845	N	SER	B	10	21.202	22.316	15.236	1.00	27.72
3846	CA	SER	B	10	20.736	20.953	15.495	1.00	27.49
3847	C	SER	B	10	20.951	20.056	14.274	1.00	27.94
3848	O	SER	B	10	21.313	18.887	14.4	1.00	25.9
3849	CB	SER	B	10	19.247	20.956	15.865	1.00	27.87
3850	OG	SER	B	10	19.005	21.672	17.061	1.00	28.12
3851	N	LEU	B	11	20.701	20.607	13.092	1.00	29.1
3852	CA	LEU	B	11	20.881	19.864	11.855	1.00	30.22
3853	C	LEU	B	11	22.358	19.522	11.683	1.00	30.91
3854	O	LEU	B	11	22.706	18.401	11.327	1.00	32.14
3855	CB	LEU	B	11	20.413	20.701	10.658	1.00	30.61
3856	CG	LEU	B	11	18.948	21.142	10.582	1.00	29.15
3857	CD1	LEU	B	11	18.785	22.146	9.455	1.00	29.01
3858	CD2	LEU	B	11	18.049	19.936	10.361	1.00	28.44
3859	N	ASN	B	12	23.221	20.498	11.946	1.00	32.43
3860	CA	ASN	B	12	24.665	20.315	11.807	1.00	33.57

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

3861	C	ASN	B	12	25.348	19.448	12.862	1.00	33.99
3862	O	ASN	B	12	26.115	18.545	12.523	1.00	34.81
3863	CB	ASN	B	12	25.386	21.669	11.796	1.00	34.56
3864	CG	ASN	B	12	25.051	22.508	10.582	1.00	36.03
3865	OD1	ASN	B	12	24.786	21.986	9.502	1.00	38.21
3866	ND2	ASN	B	12	25.085	23.821	10.75	1.00	37.59
3867	N	TYR	B	13	25.073	19.722	14.136	1.00	33.46
3868	CA	TYR	B	13	25.737	19.005	15.224	1.00	32.58
3869	C	TYR	B	13	24.868	18.199	16.176	1.00	32.32
3870	O	TYR	B	13	25.368	17.653	17.159	1.00	32.47
3871	CB	TYR	B	13	26.563	19.998	16.039	1.00	32.81
3872	CG	TYR	B	13	27.453	20.879	15.191	1.00	34.34
3873	CD1	TYR	B	13	27.219	22.249	15.093	1.00	33.8
3874	CD2	TYR	B	13	28.526	20.34	14.479	1.00	35.52
3875	CE1	TYR	B	13	28.03	23.063	14.309	1.00	35.78
3876	CE2	TYR	B	13	29.345	21.145	13.689	1.00	36.86
3877	CZ	TYR	B	13	29.092	22.505	13.611	1.00	36.86
3878	OH	TYR	B	13	29.91	23.308	12.844	1.00	38.82
3879	N	SER	B	14	23.576	18.122	15.901	1.00	31.34
3880	CA	SER	B	14	22.679	17.368	16.76	1.00	31.23
3881	C	SER	B	14	22.62	17.9	18.202	1.00	30.91
3882	O	SER	B	14	22.357	17.138	19.14	1.00	30.52
3883	CB	SER	B	14	23.095	15.896	16.774	1.00	32.78
3884	OG	SER	B	14	23.166	15.382	15.455	1.00	35.42
3885	N	VAL	B	15	22.869	19.194	18.391	1.00	29.58
3886	CA	VAL	B	15	22.792	19.756	19.738	1.00	29.64
3887	C	VAL	B	15	21.486	20.529	19.901	1.00	29.12
3888	O	VAL	B	15	20.965	21.097	18.936	1.00	30.32
3889	CB	VAL	B	15	24.001	20.685	20.067	1.00	28.91
3890	CG1	VAL	B	15	25.291	19.876	20.092	1.00	28.03
3891	CG2	VAL	B	15	24.093	21.812	19.062	1.00	28.03
3892	N	TYR	B	16	20.956	20.537	21.12	1.00	27.87
3893	CA	TYR	B	16	19.704	21.219	21.415	1.00	26.4
3894	C	TYR	B	16	19.825	22.103	22.654	1.00	26.66
3895	O	TYR	B	16	20.452	21.718	23.643	1.00	26.36
3896	CB	TYR	B	16	18.582	20.188	21.634	1.00	26.06
3897	CG	TYR	B	16	18.326	19.292	20.439	1.00	27.05
3898	CD1	TYR	B	16	19.129	18.175	20.19	1.00	25.33
3899	CD2	TYR	B	16	17.304	19.59	19.528	1.00	25.35

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

3900	CE1	TYR	B	16	18.924	17.379	19.061	1.00	27
3901	CE2	TYR	B	16	17.092	18.807	18.404	1.00	25.24
3902	CZ	TYR	B	16	17.903	17.704	18.171	1.00	27.76
3903	OH	TYR	B	16	17.689	16.938	17.048	1.00	28.5
3904	N	THR	B	17	19.211	23.284	22.592	1.00	26.55
3905	CA	THR	B	17	19.225	24.247	23.699	1.00	26.61
3906	C	THR	B	17	17.896	24.993	23.71	1.00	27.35
3907	O	THR	B	17	17.06	24.801	22.821	1.00	27.68
3908	CB	THR	B	17	20.33	25.297	23.517	1.00	26.24
3909	OG1	THR	B	17	20.029	26.094	22.366	1.00	24.14
3910	CG2	THR	B	17	21.689	24.63	23.333	1.00	24.55
3911	N	THR	B	18	17.688	25.847	24.707	1.00	28.2
3912	CA	THR	B	18	16.446	26.607	24.75	1.00	29.2
3913	C	THR	B	18	16.398	27.507	23.515	1.00	27.72
3914	O	THR	B	18	15.323	27.853	23.032	1.00	27.35
3915	CB	THR	B	18	16.336	27.465	26.027	1.00	30.01
3916	OG1	THR	B	18	17.52	28.256	26.181	1.00	34.98
3917	CG2	THR	B	18	16.181	26.584	27.235	1.00	32.23
3918	N	ASN	B	19	17.569	27.871	22.994	1.00	27.41
3919	CA	ASN	B	19	17.626	28.7	21.794	1.00	27.41
3920	C	ASN	B	19	17.113	27.934	20.568	1.00	26.8
3921	O	ASN	B	19	16.407	28.499	19.733	1.00	26.65
3922	CB	ASN	B	19	19.05	29.196	21.528	1.00	28.76
3923	CG	ASN	B	19	19.504	30.25	22.534	1.00	31.63
3924	OD1	ASN	B	19	18.748	31.154	22.89	1.00	32.34
3925	ND2	ASN	B	19	20.748	30.143	22.983	1.00	31.53
3926	N	SER	B	20	17.465	26.656	20.448	1.00	24.62
3927	CA	SER	B	20	16.987	25.88	19.313	1.00	22.43
3928	C	SER	B	20	15.487	25.615	19.492	1.00	22.59
3929	O	SER	B	20	14.769	25.419	18.516	1.00	22.32
3930	CB	SER	B	20	17.777	24.573	19.168	1.00	22.39
3931	OG	SER	B	20	17.657	23.731	20.298	1.00	20.89
3932	N	ASP	B	21	15.013	25.622	20.738	1.00	21.81
3933	CA	ASP	B	21	13.593	25.433	20.997	1.00	21.7
3934	C	ASP	B	21	12.859	26.647	20.434	1.00	22
3935	O	ASP	B	21	11.757	26.518	19.896	1.00	22.3
3936	CB	ASP	B	21	13.299	25.322	22.501	1.00	22.18
3937	CG	ASP	B	21	13.377	23.888	23.018	1.00	23.92
3938	OD1	ASP	B	21	13.437	22.948	22.194	1.00	24.05

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

3939	OD2	ASP	B	21	13.364	23.703	24.255	1.00	23.73
3940	N	VAL	B	22	13.47	27.825	20.563	1.00	21.15
3941	CA	VAL	B	22	12.864	29.052	20.05	1.00	20.55
3942	C	VAL	B	22	12.753	28.982	18.522	1.00	21.09
3943	O	VAL	B	22	11.768	29.441	17.944	1.00	21.3
3944	CB	VAL	B	22	13.675	30.305	20.486	1.00	20.84
3945	CG1	VAL	B	22	13.3	31.523	19.636	1.00	19.62
3946	CG2	VAL	B	22	13.382	30.607	21.963	1.00	20.11
3947	N	TRP	B	23	13.752	28.398	17.868	1.00	20.54
3948	CA	TRP	B	23	13.702	28.257	16.417	1.00	22.02
3949	C	TRP	B	23	12.5	27.379	16.069	1.00	22.35
3950	O	TRP	B	23	11.725	27.703	15.168	1.00	23.67
3951	CB	TRP	B	23	14.989	27.61	15.896	1.00	22.18
3952	CG	TRP	B	23	14.969	27.268	14.428	1.00	22.06
3953	CD1	TRP	B	23	14.119	26.404	13.796	1.00	21.34
3954	CD2	TRP	B	23	15.862	27.763	13.417	1.00	22.12
3955	NE1	TRP	B	23	14.428	26.328	12.459	1.00	22.22
3956	CE2	TRP	B	23	15.493	27.151	12.198	1.00	22.26
3957	CE3	TRP	B	23	16.94	28.665	13.426	1.00	22.84
3958	CZ2	TRP	B	23	16.162	27.41	10.99	1.00	24
3959	CZ3	TRP	B	23	17.609	28.927	12.223	1.00	24.89
3960	CH2	TRP	B	23	17.214	28.298	11.02	1.00	24.5
3961	N	SER	B	24	12.343	26.268	16.786	1.00	21.83
3962	CA	SER	B	24	11.22	25.373	16.54	1.00	21.88
3963	C	SER	B	24	9.91	26.095	16.831	1.00	22.36
3964	O	SER	B	24	8.911	25.886	16.136	1.00	23.47
3965	CB	SER	B	24	11.326	24.118	17.407	1.00	22.17
3966	OG	SER	B	24	12.548	23.441	17.173	1.00	22.03
3967	N	TYR	B	25	9.909	26.948	17.852	1.00	20.88
3968	CA	TYR	B	25	8.704	27.693	18.185	1.00	20.53
3969	C	TYR	B	25	8.294	28.559	16.979	1.00	20.83
3970	O	TYR	B	25	7.101	28.758	16.718	1.00	20.89
3971	CB	TYR	B	25	8.927	28.597	19.402	1.00	19.5
3972	CG	TYR	B	25	7.699	29.409	19.715	1.00	18.88
3973	CD1	TYR	B	25	6.672	28.883	20.497	1.00	19.25
3974	CD2	TYR	B	25	7.512	30.67	19.14	1.00	20.2
3975	CE1	TYR	B	25	5.479	29.592	20.695	1.00	19.78
3976	CE2	TYR	B	25	6.328	31.385	19.329	1.00	18.8
3977	CZ	TYR	B	25	5.319	30.84	20.102	1.00	19.7

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

3978	OH	TYR	B	25	4.144	31.536	20.257	1.00	21.24
3979	N	GLY	B	26	9.285	29.078	16.259	1.00	18.99
3980	CA	GLY	B	26	8.996	29.88	15.083	1.00	18.91
3981	C	GLY	B	26	8.228	29.08	14.036	1.00	19.22
3982	O	GLY	B	26	7.258	29.564	13.461	1.00	18.86
3983	N	VAL	B	27	8.672	27.852	13.788	1.00	19.32
3984	CA	VAL	B	27	8.029	26.973	12.819	1.00	19.49
3985	C	VAL	B	27	6.631	26.61	13.324	1.00	20.02
3986	O	VAL	B	27	5.697	26.442	12.542	1.00	20.61
3987	CB	VAL	B	27	8.853	25.673	12.622	1.00	19.89
3988	CG1	VAL	B	27	8.258	24.84	11.504	1.00	17.2
3989	CG2	VAL	B	27	10.318	26.023	12.304	1.00	19.05
3990	N	LEU	B	28	6.491	26.499	14.641	1.00	20.72
3991	CA	LEU	B	28	5.21	26.175	15.252	1.00	20.08
3992	C	LEU	B	28	4.221	27.331	15.018	1.00	19.23
3993	O	LEU	B	28	3.049	27.109	14.702	1.00	17.61
3994	CB	LEU	B	28	5.402	25.926	16.756	1.00	20.56
3995	CG	LEU	B	28	4.186	25.536	17.596	1.00	22.09
3996	CD1	LEU	B	28	4.645	24.91	18.908	1.00	25.1
3997	CD2	LEU	B	28	3.342	26.747	17.868	1.00	23.18
3998	N	LEU	B	29	4.699	28.56	15.185	1.00	18.17
3999	CA	LEU	B	29	3.864	29.744	14.978	1.00	19.04
4000	C	LEU	B	29	3.438	29.788	13.504	1.00	19.61
4001	O	LEU	B	29	2.321	30.2	13.173	1.00	20.78
4002	CB	LEU	B	29	4.647	31.013	15.345	1.00	18.35
4003	CG	LEU	B	29	3.95	32.363	15.118	1.00	18.58
4004	CD1	LEU	B	29	2.658	32.423	15.886	1.00	18.64
4005	CD2	LEU	B	29	4.87	33.494	15.548	1.00	17.51
4006	N	TRP	B	30	4.338	29.359	12.624	1.00	19.22
4007	CA	TRP	B	30	4.054	29.311	11.194	1.00	19.84
4008	C	TRP	B	30	2.965	28.252	10.953	1.00	20.12
4009	O	TRP	B	30	2.111	28.432	10.097	1.00	20.5
4010	CB	TRP	B	30	5.327	28.95	10.423	1.00	21.02
4011	CG	TRP	B	30	5.205	29.025	8.927	1.00	22.82
4012	CD1	TRP	B	30	5.575	30.07	8.121	1.00	23.07
4013	CD2	TRP	B	30	4.73	27.995	8.053	1.00	22.31
4014	NE1	TRP	B	30	5.366	29.747	6.8	1.00	22.96
4015	CE2	TRP	B	30	4.846	28.481	6.73	1.00	22.98
4016	CE3	TRP	B	30	4.219	26.707	8.258	1.00	21.29

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TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

4017	CZ2	TRP	B	30	4.47	27.719	5.614	1.00	23.32
4018	CZ3	TRP	B	30	3.847	25.949	7.148	1.00	22.83
4019	CH2	TRP	B	30	3.975	26.46	5.843	1.00	22.12
4020	N	GLU	B	31	2.993	27.152	11.709	1.00	20.04
4021	CA	GLU	B	31	1.97	26.112	11.561	1.00	21.34
4022	C	GLU	B	31	0.616	26.667	11.975	1.00	22.83
4023	O	GLU	B	31	-0.398	26.397	11.337	1.00	22.43
4024	CB	GLU	B	31	2.251	24.897	12.444	1.00	20.82
4025	CG	GLU	B	31	3.429	24.038	12.05	1.00	19.66
4026	CD	GLU	B	31	3.599	22.875	13.01	1.00	19.42
4027	OE1	GLU	B	31	2.951	21.82	12.81	1.00	19.39
4028	OE2	GLU	B	31	4.367	23.028	13.983	1.00	17.83
4029	N	ILE	B	32	0.602	27.428	13.064	1.00	23.29
4030	CA	ILE	B	32	-0.64	28.013	13.549	1.00	23.56
4031	C	ILE	B	32	-1.214	28.992	12.526	1.00	23.43
4032	O	ILE	B	32	-2.396	28.925	12.184	1.00	23.36
4033	CB	ILE	B	32	-0.422	28.754	14.887	1.00	22.43
4034	CG1	ILE	B	32	-0.095	27.741	15.993	1.00	23.44
4035	CG2	ILE	B	32	-1.664	29.557	15.245	1.00	21.62
4036	CD1	ILE	B	32	0.128	28.368	17.342	1.00	22.34
4037	N	VAL	B	33	-0.363	29.898	12.049	1.00	23.26
4038	CA	VAL	B	33	-0.75	30.916	11.074	1.00	23.23
4039	C	VAL	B	33	-1.258	30.296	9.771	1.00	23.6
4040	O	VAL	B	33	-2.262	30.749	9.209	1.00	23.8
4041	CB	VAL	B	33	0.45	31.86	10.757	1.00	23.24
4042	CG1	VAL	B	33	0.123	32.763	9.568	1.00	22.11
4043	CG2	VAL	B	33	0.788	32.701	11.991	1.00	23.2
4044	N	SER	B	34	-0.571	29.26	9.296	1.00	22.65
4045	CA	SER	B	34	-0.964	28.604	8.054	1.00	23.12
4046	C	SER	B	34	-2.054	27.561	8.27	1.00	23.38
4047	O	SER	B	34	-2.316	26.754	7.388	1.00	23.15
4048	CB	SER	B	34	0.246	27.944	7.399	1.00	23.15
4049	OG	SER	B	34	0.642	26.797	8.118	1.00	24.12
4050	N	LEU	B	35	-2.678	27.576	9.448	1.00	22.62
4051	CA	LEU	B	35	-3.743	26.633	9.77	1.00	22.8
4052	C	LEU	B	35	-3.368	25.159	9.57	1.00	24.05
4053	O	LEU	B	35	-4.165	24.372	9.053	1.00	24.06
4054	CB	LEU	B	35	-5.004	26.963	8.954	1.00	23.08
4055	CG	LEU	B	35	-5.572	28.385	9.111	1.00	23.52

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TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

4056	CD1	LEU	B	35	-6.728	28.605	8.14	1.00	22.66
4057	CD2	LEU	B	35	-6.046	28.599	10.546	1.00	23
4058	N	GLY	B	36	-2.158	24.785	9.984	1.00	23.75
4059	CA	GLY	B	36	-1.734	23.4	9.87	1.00	22.23
4060	C	GLY	B	36	-0.993	22.978	8.616	1.00	22.46
4061	O	GLY	B	36	-0.914	21.785	8.314	1.00	21.68
4062	N	GLY	B	37	-0.449	23.935	7.875	1.00	22.64
4063	CA	GLY	B	37	0.285	23.579	6.676	1.00	23.34
4064	C	GLY	B	37	1.605	22.908	7.013	1.00	24.36
4065	O	GLY	B	37	2.152	23.106	8.098	1.00	24.63
4066	N	THR	B	38	2.117	22.105	6.089	1.00	24.71
4067	CA	THR	B	38	3.388	21.416	6.288	1.00	25.24
4068	C	THR	B	38	4.529	22.382	5.98	1.00	24.55
4069	O	THR	B	38	4.566	22.981	4.906	1.00	25.7
4070	CB	THR	B	38	3.516	20.199	5.344	1.00	26.42
4071	OG1	THR	B	38	2.52	19.226	5.68	1.00	27.35
4072	CG2	THR	B	38	4.896	19.563	5.464	1.00	27.29
4073	N	PRO	B	39	5.471	22.552	6.921	1.00	23.53
4074	CA	PRO	B	39	6.61	23.453	6.724	1.00	23.26
4075	C	PRO	B	39	7.475	23.041	5.523	1.00	23.24
4076	O	PRO	B	39	7.803	21.867	5.359	1.00	20.79
4077	CB	PRO	B	39	7.377	23.338	8.047	1.00	23.05
4078	CG	PRO	B	39	6.311	22.977	9.039	1.00	23.62
4079	CD	PRO	B	39	5.492	21.969	8.275	1.00	23.65
4080	N	TYR	B	40	7.85	24.01	4.695	1.00	24.08
4081	CA	TYR	B	40	8.678	23.735	3.524	1.00	27.43
4082	C	TYR	B	40	7.987	22.666	2.654	1.00	29.52
4083	O	TYR	B	40	8.646	21.754	2.15	1.00	27.4
4084	CB	TYR	B	40	10.053	23.206	3.963	1.00	27.55
4085	CG	TYR	B	40	10.755	24.015	5.039	1.00	28.71
4086	CD1	TYR	B	40	11.406	25.208	4.735	1.00	28.54
4087	CD2	TYR	B	40	10.786	23.571	6.364	1.00	28.15
4088	CE1	TYR	B	40	12.075	25.941	5.721	1.00	28.53
4089	CE2	TYR	B	40	11.446	24.292	7.352	1.00	29.76
4090	CZ	TYR	B	40	12.092	25.476	7.025	1.00	29.35
4091	OH	TYR	B	40	12.753	26.189	8.003	1.00	29.37
4092	N	CYS	B	41	6.667	22.769	2.494	1.00	31.23
4093	CA	CYS	B	41	5.923	21.793	1.696	1.00	34.23
4094	C	CYS	B	41	6.512	21.674	0.292	1.00	34.6



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TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

4095	O	CYS	B	41	6.61	22.657	-0.435	1.00	33.31
4096	CB	CYS	B	41	4.444	22.184	1.603	1.00	35.2
4097	SG	CYS	B	41	3.356	20.843	1.015	1.00	39.74
4098	N	GLY	B	42	6.915	20.464	-0.076	1.00	36.64
4099	CA	GLY	B	42	7.494	20.255	-1.39	1.00	39.64
4100	C	GLY	B	42	8.999	20.049	-1.381	1.00	41.04
4101	O	GLY	B	42	9.535	19.354	-2.248	1.00	42.31
4102	N	MET	B	43	9.688	20.654	-0.418	1.00	41.55
4103	CA	MET	B	43	11.137	20.508	-0.321	1.00	41.89
4104	C	MET	B	43	11.475	19.237	0.437	1.00	41.51
4105	O	MET	B	43	10.732	18.817	1.322	1.00	41.91
4106	CB	MET	B	43	11.76	21.703	0.4	1.00	43.29
4107	CG	MET	B	43	11.638	23.019	-0.341	1.00	45.2
4108	SD	MET	B	43	12.512	24.349	0.516	1.00	48.79
4109	CE	MET	B	43	11.226	25.009	1.459	1.00	49.13
4110	N	THR	B	44	12.594	18.62	0.082	1.00	41.21
4111	CA	THR	B	44	13.021	17.397	0.746	1.00	41.54
4112	C	THR	B	44	13.896	17.753	1.933	1.00	42.27
4113	O	THR	B	44	14.315	18.903	2.083	1.00	41.87
4114	CB	THR	B	44	13.848	16.503	-0.189	1.00	41.28
4115	OG1	THR	B	44	15.048	17.19	-0.557	1.00	40.3
4116	CG2	THR	B	44	13.053	16.163	-1.446	1.00	40.82
4117	N	CYS	B	45	14.171	16.761	2.771	1.00	42.99
4118	CA	CYS	B	45	15.005	16.968	3.939	1.00	44.05
4119	C	CYS	B	45	16.424	17.285	3.491	1.00	44.24
4120	O	CYS	B	45	17.119	18.076	4.121	1.00	44.68
4121	CB	CYS	B	45	14.987	15.725	4.833	1.00	44.5
4122	SG	CYS	B	45	13.384	15.421	5.652	1.00	48.17
4123	N	ALA	B	46	16.846	16.676	2.389	1.00	44.45
4124	CA	ALA	B	46	18.185	16.91	1.865	1.00	45.29
4125	C	ALA	B	46	18.321	18.368	1.445	1.00	45.93
4126	O	ALA	B	46	19.351	19.001	1.683	1.00	45.98
4127	CB	ALA	B	46	18.455	15.986	0.673	1.00	44.48
4128	N	GLU	B	47	17.275	18.899	0.821	1.00	46.59
4129	CA	GLU	B	47	17.283	20.285	0.374	1.00	47.17
4130	C	GLU	B	47	17.354	21.243	1.556	1.00	46.77
4131	O	GLU	B	47	17.942	22.318	1.457	1.00	46.56
4132	CB	GLU	B	47	16.031	20.585	-0.45	1.00	48.68
4133	CG	GLU	B	47	15.956	19.829	-1.767	1.00	51.15

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

4134	CD	GLU	B	47	14.757	20.234	-2.607	1.00	51.73
4135	OE1	GLU	B	47	14.624	19.727	-3.74	1.00	52.77
4136	OE2	GLU	B	47	13.949	21.059	-2.136	1.00	52.46
4137	N	LEU	B	48	16.755	20.85	2.674	1.00	46.21
4138	CA	LEU	B	48	16.759	21.693	3.862	1.00	46.14
4139	C	LEU	B	48	18.145	21.772	4.491	1.00	45.94
4140	O	LEU	B	48	18.6	22.855	4.851	1.00	45.87
4141	CB	LEU	B	48	15.744	21.176	4.887	1.00	44.72
4142	CG	LEU	B	48	14.284	21.256	4.437	1.00	44.65
4143	CD1	LEU	B	48	13.378	20.644	5.497	1.00	44.42
4144	CD2	LEU	B	48	13.915	22.712	4.177	1.00	43.98
4145	N	TYR	B	49	18.812	20.628	4.623	1.00	46.36
4146	CA	TYR	B	49	20.15	20.599	5.208	1.00	46.96
4147	C	TYR	B	49	21.094	21.491	4.423	1.00	47.36
4148	O	TYR	B	49	22.066	22.009	4.963	1.00	47.66
4149	CB	TYR	B	49	20.724	19.179	5.218	1.00	45.94
4150	CG	TYR	B	49	20.302	18.328	6.391	1.00	45.32
4151	CD1	TYR	B	49	19.082	17.653	6.386	1.00	45.51
4152	CD2	TYR	B	49	21.132	18.186	7.505	1.00	45.05
4153	CE1	TYR	B	49	18.7	16.848	7.463	1.00	44.69
4154	CE2	TYR	B	49	20.758	17.388	8.585	1.00	44.24
4155	CZ	TYR	B	49	19.542	16.722	8.557	1.00	44.51
4156	OH	TYR	B	49	19.167	15.931	9.619	1.00	42.85
4157	N	GLU	B	50	20.793	21.666	3.144	1.00	48.46
4158	CA	GLU	B	50	21.618	22.476	2.259	1.00	50.31
4159	C	GLU	B	50	21.223	23.947	2.239	1.00	50.01
4160	O	GLU	B	50	22.042	24.826	2.512	1.00	50.49
4161	CB	GLU	B	50	21.537	21.914	0.839	1.00	52.81
4162	CG	GLU	B	50	22.078	22.837	-0.236	1.00	57.04
4163	CD	GLU	B	50	21.589	22.453	-1.619	1.00	59.86
4164	OE1	GLU	B	50	21.896	21.327	-2.069	1.00	61.53
4165	OE2	GLU	B	50	20.89	23.275	-2.254	1.00	61.58
4166	N	LYS	B	51	19.963	24.203	1.907	1.00	49.14
4167	CA	LYS	B	51	19.444	25.56	1.806	1.00	48.32
4168	C	LYS	B	51	19.46	26.371	3.097	1.00	46.75
4169	O	LYS	B	51	19.917	27.514	3.103	1.00	45.93
4170	CB	LYS	B	51	18.017	25.523	1.257	1.00	49.88
4171	CG	LYS	B	51	17.886	24.918	-0.129	1.00	52.22
4172	CD	LYS	B	51	18.454	25.841	-1.19	1.00	54.79

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

4173	CE	LYS	B	51	18.216	25.284	-2.586	1.00	55.63
4174	NZ	LYS	B	51	18.751	26.203	-3.631	1.00	56.77
4175	N	LEU	B	52	18.957	25.792	4.185	1.00	45.62
4176	CA	LEU	B	52	18.897	26.502	5.464	1.00	45.04
4177	C	LEU	B	52	20.196	27.192	5.881	1.00	44.93
4178	O	LEU	B	52	20.197	28.385	6.175	1.00	44.01
4179	CB	LEU	B	52	18.417	25.564	6.577	1.00	43.65
4180	CG	LEU	B	52	16.96	25.106	6.457	1.00	43.95
4181	CD1	LEU	B	52	16.596	24.273	7.673	1.00	44.28
4182	CD2	LEU	B	52	16.033	26.31	6.352	1.00	43.25
4183	N	PRO	B	53	21.318	26.455	5.918	1.00	45.8
4184	CA	PRO	B	53	22.578	27.097	6.313	1.00	45.97
4185	C	PRO	B	53	22.962	28.26	5.394	1.00	45.81
4186	O	PRO	B	53	23.742	29.132	5.776	1.00	46.35
4187	CB	PRO	B	53	23.585	25.947	6.248	1.00	45.99
4188	CG	PRO	B	53	22.747	24.753	6.614	1.00	46.19
4189	CD	PRO	B	53	21.491	24.996	5.795	1.00	46.16
4190	N	GLN	B	54	22.405	28.276	4.186	1.00	45
4191	CA	GLN	B	54	22.705	29.33	3.226	1.00	44.05
4192	C	GLN	B	54	21.886	30.602	3.447	1.00	42.69
4193	O	GLN	B	54	22.11	31.612	2.774	1.00	42.32
4194	CB	GLN	B	54	22.472	28.822	1.807	1.00	45.86
4195	CG	GLN	B	54	23.243	27.563	1.459	1.00	48.82
4196	CD	GLN	B	54	22.85	27.011	0.098	1.00	50.8
4197	OE1	GLN	B	54	23.293	25.933	-0.302	1.00	52
4198	NE2	GLN	B	54	22.013	27.754	-0.624	1.00	51.7
4199	N	GLY	B	55	20.936	30.555	4.377	1.00	40.57
4200	CA	GLY	B	55	20.126	31.728	4.653	1.00	38.2
4201	C	GLY	B	55	18.656	31.575	4.303	1.00	37.79
4202	O	GLY	B	55	17.851	32.466	4.586	1.00	37.04
4203	N	TYR	B	56	18.297	30.45	3.692	1.00	36.36
4204	CA	TYR	B	56	16.91	30.209	3.315	1.00	35.73
4205	C	TYR	B	56	15.992	30.024	4.526	1.00	34.27
4206	O	TYR	B	56	16.341	29.341	5.489	1.00	33.69
4207	CB	TYR	B	56	16.814	28.981	2.402	1.00	36.35
4208	CG	TYR	B	56	15.406	28.696	1.929	1.00	38.54
4209	CD1	TYR	B	56	14.564	27.849	2.649	1.00	38.66
4210	CD2	TYR	B	56	14.901	29.308	0.781	1.00	39.21
4211	CE1	TYR	B	56	13.253	27.619	2.239	1.00	39.55

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

4212	CE2	TYR	B	56	13.59	29.086	0.362	1.00	40.19
4213	CZ	TYR	B	56	12.773	28.241	1.096	1.00	40.5
4214	OH	TYR	B	56	11.475	28.028	0.691	1.00	41.85
4215	N	ARG	B	57	14.816	30.641	4.466	1.00	32.76
4216	CA	ARG	B	57	13.836	30.54	5.546	1.00	31.77
4217	C	ARG	B	57	12.428	30.4	4.977	1.00	31.42
4218	O	ARG	B	57	12.173	30.756	3.825	1.00	30.09
4219	CB	ARG	B	57	13.878	31.788	6.43	1.00	30.74
4220	CG	ARG	B	57	15.187	32.009	7.165	1.00	31.13
4221	CD	ARG	B	57	15.414	30.96	8.241	1.00	29.93
4222	NE	ARG	B	57	16.606	31.263	9.029	1.00	31.37
4223	CZ	ARG	B	57	17.852	31.007	8.64	1.00	31.81
4224	NH1	ARG	B	57	18.078	30.429	7.465	1.00	30.33
4225	NH2	ARG	B	57	18.875	31.344	9.421	1.00	31.58
4226	N	LEU	B	58	11.517	29.876	5.79	1.00	30.93
4227	CA	LEU	B	58	10.128	29.729	5.377	1.00	31.14
4228	C	LEU	B	58	9.607	31.089	4.924	1.00	31.68
4229	O	LEU	B	58	10.012	32.131	5.44	1.00	31.2
4230	CB	LEU	B	58	9.263	29.243	6.54	1.00	29.55
4231	CG	LEU	B	58	9.388	27.8	7.012	1.00	30.01
4232	CD1	LEU	B	58	8.716	27.661	8.378	1.00	29.28
4233	CD2	LEU	B	58	8.748	26.865	5.987	1.00	29.33
4234	N	GLU	B	59	8.695	31.07	3.966	1.00	32.57
4235	CA	GLU	B	59	8.119	32.295	3.451	1.00	33.63
4236	C	GLU	B	59	6.877	32.678	4.239	1.00	32.08
4237	O	GLU	B	59	6.242	31.833	4.872	1.00	31.36
4238	CB	GLU	B	59	7.806	32.124	1.961	1.00	36.89
4239	CG	GLU	B	59	9.07	32.173	1.11	1.00	42.49
4240	CD	GLU	B	59	8.983	31.338	-0.148	1.00	46.28
4241	OE1	GLU	B	59	8.081	31.581	-0.975	1.00	48.52
4242	OE2	GLU	B	59	9.83	30.432	-0.311	1.00	49.56
4243	N	LYS	B	60	6.553	33.966	4.215	1.00	30.81
4244	CA	LYS	B	60	5.397	34.483	4.927	1.00	30.12
4245	C	LYS	B	60	4.08	33.973	4.356	1.00	29.5
4246	O	LYS	B	60	3.809	34.13	3.17	1.00	29.01
4247	CB	LYS	B	60	5.402	36.009	4.884	1.00	30.46
4248	CG	LYS	B	60	4.264	36.644	5.667	1.00	31.07
4249	CD	LYS	B	60	4.398	38.155	5.716	1.00	32.26
4250	CE	LYS	B	60	3.988	38.804	4.413	1.00	34.38

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

4251	NZ	LYS	B	60	2.531	38.596	4.153	1.00	37.08
4252	N	PRO	B	61	3.248	33.341	5.196	1.00	29.47
4253	CA	PRO	B	61	1.957	32.832	4.715	1.00	29.32
4254	C	PRO	B	61	1.164	34	4.118	1.00	29.96
4255	O	PRO	B	61	1.331	35.144	4.538	1.00	30.22
4256	CB	PRO	B	61	1.315	32.276	5.981	1.00	29.4
4257	CG	PRO	B	61	2.505	31.819	6.782	1.00	29.51
4258	CD	PRO	B	61	3.488	32.951	6.596	1.00	28.84
4259	N	LEU	B	62	0.296	33.72	3.154	1.00	30.35
4260	CA	LEU	B	62	-0.469	34.784	2.501	1.00	31.05
4261	C	LEU	B	62	-1.48	35.522	3.388	1.00	29.91
4262	O	LEU	B	62	-1.926	36.613	3.047	1.00	31.75
4263	CB	LEU	B	62	-1.179	34.217	1.268	1.00	32.13
4264	CG	LEU	B	62	-0.262	33.51	0.264	1.00	34.14
4265	CD1	LEU	B	62	-1.089	32.87	-0.848	1.00	34.11
4266	CD2	LEU	B	62	0.725	34.512	-0.312	1.00	34.34
4267	N	ASN	B	63	-1.832	34.94	4.526	1.00	28.19
4268	CA	ASN	B	63	-2.802	35.556	5.429	1.00	26.63
4269	C	ASN	B	63	-2.107	36.1	6.679	1.00	26.12
4270	O	ASN	B	63	-2.758	36.435	7.662	1.00	27.46
4271	CB	ASN	B	63	-3.835	34.506	5.85	1.00	24.86
4272	CG	ASN	B	63	-3.208	33.366	6.645	1.00	23.63
4273	OD1	ASN	B	63	-2.138	32.874	6.295	1.00	23.85
4274	ND2	ASN	B	63	-3.87	32.946	7.717	1.00	23.26
4275	N	CYS	B	64	-0.788	36.199	6.63	1.00	25.92
4276	CA	CYS	B	64	-0.013	36.642	7.781	1.00	25.93
4277	C	CYS	B	64	0.434	38.103	7.774	1.00	26.08
4278	O	CYS	B	64	1.051	38.56	6.822	1.00	25.66
4279	CB	CYS	B	64	1.215	35.738	7.916	1.00	24.78
4280	SG	CYS	B	64	2.201	35.99	9.404	1.00	26.2
4281	N	ASP	B	65	0.138	38.826	8.851	1.00	26.7
4282	CA	ASP	B	65	0.555	40.22	8.951	1.00	28.84
4283	C	ASP	B	65	2.078	40.243	9.026	1.00	29.2
4284	O	ASP	B	65	2.69	39.297	9.52	1.00	29.25
4285	CB	ASP	B	65	-0.006	40.879	10.215	1.00	30.53
4286	CG	ASP	B	65	0.311	42.367	10.279	1.00	32.84
4287	OD1	ASP	B	65	-0.396	43.149	9.614	1.00	34.64
4288	OD2	ASP	B	65	1.275	42.758	10.973	1.00	35.12
4289	N	ASP	B	66	2.689	41.323	8.547	1.00	29.01

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

4290	CA	ASP	B	66	4.142	41.44	8.575	1.00	29.59
4291	C	ASP	B	66	4.747	41.344	9.973	1.00	28.75
4292	O	ASP	B	66	5.855	40.835	10.135	1.00	27.93
4293	CB	ASP	B	66	4.595	42.763	7.948	1.00	32.52
4294	CG	ASP	B	66	4.382	42.804	6.449	1.00	34.61
4295	OD1	ASP	B	66	4.677	41.798	5.771	1.00	36.77
4296	OD2	ASP	B	66	3.932	43.849	5.944	1.00	37.27
4297	N	GLU	B	67	4.037	41.831	10.985	1.00	28.17
4298	CA	GLU	B	67	4.583	41.79	12.339	1.00	28.49
4299	C	GLU	B	67	4.704	40.36	12.869	1.00	27.64
4300	O	GLU	B	67	5.661	40.032	13.567	1.00	28.63
4301	CB	GLU	B	67	3.728	42.632	13.293	1.00	30.2
4302	CG	GLU	B	67	4.504	43.109	14.519	1.00	31.89
4303	CD	GLU	B	67	3.632	43.792	15.565	1.00	32.22
4304	OE1	GLU	B	67	2.573	44.352	15.208	1.00	30.69
4305	OE2	GLU	B	67	4.024	43.776	16.751	1.00	32.36
4306	N	VAL	B	68	3.74	39.507	12.536	1.00	26.85
4307	CA	VAL	B	68	3.785	38.119	12.983	1.00	25.57
4308	C	VAL	B	68	4.932	37.404	12.278	1.00	24.86
4309	O	VAL	B	68	5.632	36.581	12.873	1.00	24.44
4310	CB	VAL	B	68	2.468	37.363	12.667	1.00	25.44
4311	CG1	VAL	B	68	2.555	35.942	13.186	1.00	25.25
4312	CG2	VAL	B	68	1.276	38.075	13.312	1.00	25.17
4313	N	TYR	B	69	5.125	37.725	11.004	1.00	24.96
4314	CA	TYR	B	69	6.184	37.105	10.223	1.00	24.53
4315	C	TYR	B	69	7.561	37.521	10.734	1.00	25.4
4316	O	TYR	B	69	8.489	36.711	10.775	1.00	25.92
4317	CB	TYR	B	69	6.049	37.474	8.742	1.00	22.82
4318	CG	TYR	B	69	7.059	36.763	7.873	1.00	21.6
4319	CD1	TYR	B	69	7.101	35.376	7.826	1.00	21.11
4320	CD2	TYR	B	69	7.984	37.475	7.113	1.00	21.11
4321	CE1	TYR	B	69	8.037	34.704	7.045	1.00	21.45
4322	CE2	TYR	B	69	8.931	36.813	6.325	1.00	22.15
4323	CZ	TYR	B	69	8.949	35.428	6.3	1.00	22.19
4324	OH	TYR	B	69	9.881	34.757	5.545	1.00	23.63
4325	N	ASP	B	70	7.695	38.786	11.117	1.00	26.04
4326	CA	ASP	B	70	8.968	39.269	11.636	1.00	28.23
4327	C	ASP	B	70	9.302	38.548	12.95	1.00	27.55
4328	O	ASP	B	70	10.469	38.314	13.259	1.00	27.34

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

4329	CB	ASP	B	70	8.923	40.78	11.877	1.00	31.33
4330	CG	ASP	B	70	10.237	41.31	12.42	1.00	36.14
4331	OD1	ASP	B	70	11.271	41.148	11.729	1.00	38.15
4332	OD2	ASP	B	70	10.243	41.872	13.54	1.00	38.77
4333	N	LEU	B	71	8.273	38.21	13.723	1.00	25.5
4334	CA	LEU	B	71	8.472	37.499	14.971	1.00	24.2
4335	C	LEU	B	71	9.05	36.134	14.6	1.00	24.61
4336	O	LEU	B	71	10.009	35.666	15.216	1.00	24.66
4337	CB	LEU	B	71	7.142	37.352	15.715	1.00	23.27
4338	CG	LEU	B	71	7.151	36.582	17.04	1.00	24.33
4339	CD1	LEU	B	71	8.307	37.061	17.931	1.00	23.68
4340	CD2	LEU	B	71	5.803	36.776	17.74	1.00	23.11
4341	N	MET	B	72	8.465	35.504	13.585	1.00	23.43
4342	CA	MET	B	72	8.95	34.212	13.099	1.00	23.68
4343	C	MET	B	72	10.423	34.323	12.703	1.00	24.01
4344	O	MET	B	72	11.244	33.486	13.077	1.00	24.21
4345	CB	MET	B	72	8.163	33.759	11.859	1.00	22.23
4346	CG	MET	B	72	6.793	33.179	12.13	1.00	22.37
4347	SD	MET	B	72	5.966	32.72	10.577	1.00	24.06
4348	CE	MET	B	72	4.28	33.249	10.909	1.00	23.74
4349	N	ARG	B	73	10.741	35.359	11.93	1.00	25.23
4350	CA	ARG	B	73	12.103	35.582	11.462	1.00	26.57
4351	C	ARG	B	73	13.104	35.786	12.602	1.00	26.61
4352	O	ARG	B	73	14.263	35.391	12.486	1.00	25.99
4353	CB	ARG	B	73	12.136	36.77	10.489	1.00	27.99
4354	CG	ARG	B	73	11.29	36.548	9.219	1.00	29.53
4355	CD	ARG	B	73	11.707	35.28	8.472	1.00	29.11
4356	NE	ARG	B	73	13.086	35.357	7.99	1.00	32.97
4357	CZ	ARG	B	73	13.45	35.836	6.801	1.00	33.65
4358	NH1	ARG	B	73	12.539	36.28	5.948	1.00	33.99
4359	NH2	ARG	B	73	14.732	35.887	6.472	1.00	34.28
4360	N	GLN	B	74	12.657	36.387	13.702	1.00	26.32
4361	CA	GLN	B	74	13.532	36.598	14.856	1.00	26.67
4362	C	GLN	B	74	13.942	35.232	15.426	1.00	26.47
4363	O	GLN	B	74	15.097	35.038	15.821	1.00	26.58
4364	CB	GLN	B	74	12.812	37.396	15.952	1.00	28.56
4365	CG	GLN	B	74	12.29	38.768	15.536	1.00	32.23
4366	CD	GLN	B	74	11.467	39.445	16.637	1.00	35.89
4367	OE1	GLN	B	74	10.709	40.394	16.379	1.00	36.27

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

4368	NE2	GLN	B	74	11.62	38.964	17.871	1.00	35.72
4369	N	CYS	B	75	12.992	34.294	15.461	1.00	23.81
4370	CA	CYS	B	75	13.244	32.954	15.987	1.00	23.07
4371	C	CYS	B	75	14.211	32.127	15.136	1.00	22.4
4372	O	CYS	B	75	14.813	31.175	15.634	1.00	20.39
4373	CB	CYS	B	75	11.923	32.175	16.135	1.00	23.16
4374	SG	CYS	B	75	10.656	32.914	17.235	1.00	23.14
4375	N	TRP	B	76	14.376	32.492	13.865	1.00	23.37
4376	CA	TRP	B	76	15.262	31.734	12.979	1.00	23.97
4377	C	TRP	B	76	16.592	32.409	12.641	1.00	25.54
4378	O	TRP	B	76	17.218	32.093	11.617	1.00	24.48
4379	CB	TRP	B	76	14.535	31.383	11.675	1.00	24.03
4380	CG	TRP	B	76	13.195	30.745	11.884	1.00	24.4
4381	CD1	TRP	B	76	12.868	29.811	12.827	1.00	22.28
4382	CD2	TRP	B	76	12.009	30.968	11.111	1.00	24.33
4383	NE1	TRP	B	76	11.554	29.439	12.687	1.00	22.24
4384	CE2	TRP	B	76	11.002	30.133	11.642	1.00	23.98
4385	CE3	TRP	B	76	11.7	31.791	10.019	1.00	24.23
4386	CZ2	TRP	B	76	9.702	30.099	11.12	1.00	24.17
4387	CZ3	TRP	B	76	10.408	31.757	9.499	1.00	25.59
4388	CH2	TRP	B	76	9.425	30.913	10.052	1.00	24.6
4389	N	ARG	B	77	17.025	33.333	13.494	1.00	26.57
4390	CA	ARG	B	77	18.294	34.021	13.273	1.00	28.95
4391	C	ARG	B	77	19.407	32.987	13.367	1.00	29.71
4392	O	ARG	B	77	19.377	32.11	14.229	1.00	28.67
4393	CB	ARG	B	77	18.485	35.124	14.318	1.00	30.04
4394	CG	ARG	B	77	17.633	36.355	14.049	1.00	33.2
4395	CD	ARG	B	77	17.493	37.244	15.272	1.00	35.61
4396	NE	ARG	B	77	16.801	38.489	14.939	1.00	39.33
4397	CZ	ARG	B	77	16.265	39.318	15.831	1.00	39.45
4398	NH1	ARG	B	77	15.658	40.426	15.422	1.00	39.08
4399	NH2	ARG	B	77	16.322	39.034	17.128	1.00	38.75
4400	N	GLU	B	78	20.381	33.084	12.471	1.00	31.85
4401	CA	GLU	B	78	21.484	32.132	12.443	1.00	34.78
4402	C	GLU	B	78	22.147	31.939	13.803	1.00	34.45
4403	O	GLU	B	78	22.297	30.811	14.267	1.00	33.85
4404	CB	GLU	B	78	22.532	32.568	11.42	1.00	37.54
4405	CG	GLU	B	78	23.488	31.459	11.031	1.00	43.97
4406	CD	GLU	B	78	24.567	31.93	10.077	1.00	48.2



TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

4407	OE1	GLU	B	78	24.442	33.055	9.541	1.00	50.7
4408	OE2	GLU	B	78	25.535	31.17	9.857	1.00	50.48
4409	N	LYS	B	79	22.547	33.036	14.437	1.00	34.82
4410	CA	LYS	B	79	23.189	32.966	15.748	1.00	36.1
4411	C	LYS	B	79	22.135	32.704	16.821	1.00	34.95
4412	O	LYS	B	79	21.209	33.494	17.002	1.00	35.2
4413	CB	LYS	B	79	23.922	34.271	16.039	1.00	38.13
4414	CG	LYS	B	79	24.99	34.608	15.015	1.00	41.47
4415	CD	LYS	B	79	25.475	36.034	15.21	1.00	44.19
4416	CE	LYS	B	79	26.569	36.394	14.221	1.00	45.34
4417	NZ	LYS	B	79	26.931	37.834	14.34	1.00	46.95
4418	N	PRO	B	80	22.269	31.588	17.548	1.00	34.32
4419	CA	PRO	B	80	21.325	31.209	18.603	1.00	33.93
4420	C	PRO	B	80	21.036	32.298	19.63	1.00	34.45
4421	O	PRO	B	80	19.893	32.466	20.053	1.00	34.71
4422	CB	PRO	B	80	21.99	29.988	19.234	1.00	33.84
4423	CG	PRO	B	80	22.73	29.376	18.084	1.00	33.41
4424	CD	PRO	B	80	23.346	30.588	17.425	1.00	33.37
4425	N	TYR	B	81	22.074	33.03	20.026	1.00	34.7
4426	CA	TYR	B	81	21.942	34.09	21.02	1.00	35.95
4427	C	TYR	B	81	21.297	35.378	20.495	1.00	36.42
4428	O	TYR	B	81	21.095	36.325	21.255	1.00	36.09
4429	CB	TYR	B	81	23.316	34.395	21.636	1.00	37.44
4430	CG	TYR	B	81	24.405	34.685	20.622	1.00	38.74
4431	CD1	TYR	B	81	24.6	35.973	20.12	1.00	40.03
4432	CD2	TYR	B	81	25.229	33.662	20.149	1.00	39.3
4433	CE1	TYR	B	81	25.591	36.236	19.173	1.00	40.71
4434	CE2	TYR	B	81	26.216	33.91	19.206	1.00	40.38
4435	CZ	TYR	B	81	26.395	35.197	18.721	1.00	41.45
4436	OH	TYR	B	81	27.38	35.439	17.787	1.00	43.15
4437	N	GLU	B	82	20.972	35.412	19.205	1.00	36.39
4438	CA	GLU	B	82	20.325	36.577	18.605	1.00	36.39
4439	C	GLU	B	82	18.81	36.409	18.702	1.00	34.12
4440	O	GLU	B	82	18.063	37.382	18.654	1.00	33.39
4441	CB	GLU	B	82	20.69	36.704	17.123	1.00	40.92
4442	CG	GLU	B	82	22.164	36.874	16.805	1.00	45.64
4443	CD	GLU	B	82	22.625	38.304	16.919	1.00	47.36
4444	OE1	GLU	B	82	23.587	38.672	16.208	1.00	48.58
4445	OE2	GLU	B	82	22.03	39.055	17.723	1.00	49.71

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

4446	N	ARG	B	83	18.362	35.164	18.818	1.00	31.77
4447	CA	ARG	B	83	16.937	34.874	18.902	1.00	29.75
4448	C	ARG	B	83	16.322	35.399	20.198	1.00	28.57
4449	O	ARG	B	83	16.99	35.5	21.226	1.00	29.33
4450	CB	ARG	B	83	16.706	33.362	18.788	1.00	29.06
4451	CG	ARG	B	83	17.332	32.756	17.542	1.00	28.35
4452	CD	ARG	B	83	17.407	31.238	17.586	1.00	25.75
4453	NE	ARG	B	83	18.348	30.77	16.574	1.00	26.14
4454	CZ	ARG	B	83	18.83	29.534	16.491	1.00	25.34
4455	NH1	ARG	B	83	18.462	28.606	17.365	1.00	25.24
4456	NH2	ARG	B	83	19.707	29.235	15.541	1.00	23.54
4457	N	PRO	B	84	15.034	35.76	20.159	1.00	27.1
4458	CA	PRO	B	84	14.4	36.262	21.378	1.00	25.38
4459	C	PRO	B	84	14.19	35.13	22.372	1.00	24.85
4460	O	PRO	B	84	14.353	33.952	22.036	1.00	23.83
4461	CB	PRO	B	84	13.083	36.831	20.868	1.00	25.65
4462	CG	PRO	B	84	12.765	35.923	19.704	1.00	25.69
4463	CD	PRO	B	84	14.104	35.811	19.017	1.00	26.3
4464	N	SER	B	85	13.842	35.496	23.601	1.00	23.92
4465	CA	SER	B	85	13.58	34.517	24.643	1.00	23.26
4466	C	SER	B	85	12.076	34.286	24.607	1.00	22.97
4467	O	SER	B	85	11.346	35.067	24	1.00	22.16
4468	CB	SER	B	85	13.974	35.076	26.008	1.00	22.27
4469	OG	SER	B	85	13.174	36.202	26.328	1.00	21.97
4470	N	PHE	B	86	11.604	33.231	25.26	1.00	22.49
4471	CA	PHE	B	86	10.174	32.968	25.264	1.00	23.47
4472	C	PHE	B	86	9.417	34.085	25.964	1.00	23.38
4473	O	PHE	B	86	8.264	34.372	25.63	1.00	23.52
4474	CB	PHE	B	86	9.879	31.601	25.904	1.00	23.41
4475	CG	PHE	B	86	10.193	30.437	24.998	1.00	22.06
4476	CD1	PHE	B	86	9.483	30.26	23.806	1.00	21.93
4477	CD2	PHE	B	86	11.221	29.548	25.307	1.00	23.03
4478	CE1	PHE	B	86	9.793	29.214	22.925	1.00	22.41
4479	CE2	PHE	B	86	11.547	28.494	24.437	1.00	23.63
4480	CZ	PHE	B	86	10.827	28.329	23.24	1.00	25.27
4481	N	ALA	B	87	10.07	34.734	26.92	1.00	24.27
4482	CA	ALA	B	87	9.435	35.839	27.639	1.00	24.29
4483	C	ALA	B	87	9.23	37.027	26.697	1.00	24.13
4484	O	ALA	B	87	8.21	37.706	26.756	1.00	24.04

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

4485	CB	ALA	B	87	10.293	36.258	28.845	1.00	24.68
4486	N	GLN	B	88	10.201	37.285	25.828	1.00	24.52
4487	CA	GLN	B	88	10.072	38.397	24.89	1.00	25.48
4488	C	GLN	B	88	9.008	38.073	23.838	1.00	25.49
4489	O	GLN	B	88	8.208	38.943	23.456	1.00	26.9
4490	CB	GLN	B	88	11.422	38.699	24.221	1.00	26.2
4491	CG	GLN	B	88	12.489	39.202	25.197	1.00	26.89
4492	CD	GLN	B	88	13.852	39.371	24.55	1.00	28.96
4493	OE1	GLN	B	88	14.329	38.482	23.845	1.00	28.16
4494	NE2	GLN	B	88	14.494	40.512	24.797	1.00	29.5
4495	N	ILE	B	89	8.995	36.82	23.386	1.00	24.1
4496	CA	ILE	B	89	8.024	36.357	22.4	1.00	22.92
4497	C	ILE	B	89	6.612	36.559	22.943	1.00	23.29
4498	O	ILE	B	89	5.715	37	22.22	1.00	23.49
4499	CB	ILE	B	89	8.242	34.85	22.07	1.00	23.28
4500	CG1	ILE	B	89	9.575	34.674	21.338	1.00	21.29
4501	CG2	ILE	B	89	7.087	34.301	21.206	1.00	20.46
4502	CD1	ILE	B	89	9.965	33.225	21.126	1.00	22.43
4503	N	LEU	B	90	6.427	36.247	24.223	1.00	22.89
4504	CA	LEU	B	90	5.131	36.385	24.866	1.00	24.53
4505	C	LEU	B	90	4.706	37.848	24.963	1.00	25.61
4506	O	LEU	B	90	3.522	38.173	24.83	1.00	25.8
4507	CB	LEU	B	90	5.164	35.759	26.261	1.00	24.36
4508	CG	LEU	B	90	3.836	35.785	27.024	1.00	26.52
4509	CD1	LEU	B	90	2.726	35.168	26.175	1.00	23.71
4510	CD2	LEU	B	90	3.995	35.025	28.332	1.00	26.22
4511	N	VAL	B	91	5.67	38.732	25.201	1.00	26.17
4512	CA	VAL	B	91	5.367	40.155	25.286	1.00	26.16
4513	C	VAL	B	91	4.887	40.646	23.918	1.00	26.04
4514	O	VAL	B	91	3.93	41.419	23.827	1.00	25.62
4515	CB	VAL	B	91	6.607	40.977	25.72	1.00	26.42
4516	CG1	VAL	B	91	6.37	42.458	25.443	1.00	26.95
4517	CG2	VAL	B	91	6.874	40.768	27.212	1.00	24.3
4518	N	SER	B	92	5.552	40.188	22.86	1.00	24.24
4519	CA	SER	B	92	5.184	40.584	21.509	1.00	24.86
4520	C	SER	B	92	3.783	40.093	21.168	1.00	25.1
4521	O	SER	B	92	2.974	40.841	20.628	1.00	25.19
4522	CB	SER	B	92	6.186	40.026	20.498	1.00	24.3
4523	OG	SER	B	92	7.502	40.443	20.821	1.00	28.32

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

4524	N	LEU	B	93	3.493	38.835	21.497	1.00	25.15
4525	CA	LEU	B	93	2.181	38.271	21.21	1.00	24.94
4526	C	LEU	B	93	1.088	39.026	21.969	1.00	25.79
4527	O	LEU	B	93	0.033	39.35	21.413	1.00	22.85
4528	CB	LEU	B	93	2.155	36.781	21.576	1.00	24.02
4529	CG	LEU	B	93	3.066	35.895	20.72	1.00	23.67
4530	CD1	LEU	B	93	3.049	34.48	21.253	1.00	22.39
4531	CD2	LEU	B	93	2.599	35.934	19.262	1.00	21.69
4532	N	ASN	B	94	1.354	39.308	23.24	1.00	26.18
4533	CA	ASN	B	94	0.398	40.026	24.071	1.00	27.68
4534	C	ASN	B	94	0.122	41.433	23.541	1.00	27.87
4535	O	ASN	B	94	-0.997	41.936	23.646	1.00	26.36
4536	CB	ASN	B	94	0.911	40.079	25.51	1.00	28.36
4537	CG	ASN	B	94	0.693	38.769	26.252	1.00	28.76
4538	OD1	ASN	B	94	1.304	38.516	27.285	1.00	31.37
4539	ND2	ASN	B	94	-0.197	37.938	25.731	1.00	28.86
4540	N	ARG	B	95	1.135	42.067	22.963	1.00	28.03
4541	CA	ARG	B	95	0.94	43.405	22.416	1.00	30.19
4542	C	ARG	B	95	-0.019	43.359	21.229	1.00	31.55
4543	O	ARG	B	95	-0.934	44.186	21.124	1.00	31.79
4544	CB	ARG	B	95	2.282	44.019	21.995	1.00	30.11
4545	CG	ARG	B	95	3.135	44.431	23.18	1.00	29.56
4546	CD	ARG	B	95	4.394	45.152	22.76	1.00	30.76
4547	NE	ARG	B	95	5.071	45.734	23.917	1.00	31.94
4548	CZ	ARG	B	95	6.155	46.502	23.846	1.00	32.96
4549	NH1	ARG	B	95	6.695	46.784	22.666	1.00	31.46
4550	NH2	ARG	B	95	6.691	47	24.956	1.00	32.31
4551	N	MET	B	96	0.18	42.385	20.344	1.00	31.77
4552	CA	MET	B	96	-0.688	42.249	19.177	1.00	33.45
4553	C	MET	B	96	-2.098	41.898	19.629	1.00	34
4554	O	MET	B	96	-3.076	42.444	19.116	1.00	34.06
4555	CB	MET	B	96	-3.156	41.173	18.223	1.00	33.52
4556	CG	MET	B	96	1.187	41.518	17.589	1.00	35.55
4557	SD	MET	B	96	1.948	40.116	16.721	1.00	36.97
4558	CE	MET	B	96	2.054	40.722	15.114	1.00	36
4559	N	LEU	B	97	-2.199	40.995	20.602	1.00	35.15
4560	CA	LEU	B	97	-3.498	40.578	21.122	1.00	37.36
4561	C	LEU	B	97	-4.281	41.753	21.702	1.00	39.63
4562	O	LEU	B	97	-5.475	41.903	21.444	1.00	38.49

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

4563	CB	LEU	B	97	-3.32	39.5	22.201	1.00	35.87
4564	CG	LEU	B	97	-2.972	38.089	21.712	1.00	35.45
4565	CD1	LEU	B	97	-2.631	37.191	22.895	1.00	34.5
4566	CD2	LEU	B	97	-4.15	37.524	20.919	1.00	34.25
4567	N	GLU	B	98	-3.591	42.585	22.473	1.00	43.11
4568	CA	GLU	B	98	-4.189	43.745	23.123	1.00	47.52
4569	C	GLU	B	98	-5.008	44.648	22.2	1.00	48.88
4570	O	GLU	B	98	-6.044	45.176	22.603	1.00	48.98
4571	CB	GLU	B	98	-3.098	44.572	23.798	1.00	50.24
4572	CG	GLU	B	98	-3.623	45.714	24.645	1.00	56.23
4573	CD	GLU	B	98	-4.431	45.226	25.834	1.00	59.79
4574	OE1	GLU	B	98	-3.92	44.366	26.586	1.00	61.53
4575	OE2	GLU	B	98	-5.571	45.705	26.019	1.00	61.71
4576	N	GLU	B	99	-4.547	44.832	20.969	1.00	50.19
4577	CA	GLU	B	99	-5.266	45.683	20.031	1.00	52.23
4578	C	GLU	B	99	-6.204	44.904	19.114	1.00	52.75
4579	O	GLU	B	99	-5.948	43.749	18.78	1.00	53.71
4580	CB	GLU	B	99	-4.273	46.522	19.218	1.00	53.54
4581	CG	GLU	B	99	-3.048	45.776	18.713	1.00	54.85
4582	CD	GLU	B	99	-1.855	46.703	18.512	1.00	55.72
4583	OE1	GLU	B	99	-0.87	46.292	17.866	1.00	56.82
4584	OE2	GLU	B	99	-1.898	47.844	19.012	1.00	55.91
4585	N	ALA	B	100	-7.305	45.538	18.725	1.00	53.06
4586	CA	ALA	B	100	-8.287	44.899	17.855	1.00	53.31
4587	C	ALA	B	100	-7.602	44.26	16.652	1.00	52.83
4588	O	ALA	B	100	-7.572	43.04	16.53	1.00	53
4589	CB	ALA	B	100	-9.324	45.922	17.39	1.00	53.49
4590	N	LYS	B	101	-7.048	45.107	15.786	1.00	52.06
4591	CA	LYS	B	101	-6.346	44.699	14.565	1.00	50.58
4592	C	LYS	B	101	-6.196	43.194	14.314	1.00	48.57
4593	O	LYS	B	101	-5.806	42.434	15.198	1.00	49.46
4594	CB	LYS	B	101	-4.959	45.358	14.524	1.00	51.23
4595	CG	LYS	B	101	-4.197	45.109	13.23	1.00	52.16
4596	CD	LYS	B	101	-2.878	45.868	13.182	1.00	53.27
4597	CE	LYS	B	101	-2.154	45.605	11.867	1.00	54.22
4598	NZ	LYS	B	101	-0.862	46.337	11.768	1.00	55.51
4599	N	THR	B	102	-6.506	42.781	13.088	1.00	45.64
4600	CA	THR	B	102	-6.403	41.385	12.678	1.00	42.49
4601	C	THR	B	102	-4.966	41.099	12.239	1.00	40.7

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

4602	O	THR	B	102	-4.461	41.745	11.321	1.00	41.62
4603	CB	THR	B	102	-7.343	41.096	11.491	1.00	42.45
4604	OG1	THR	B	102	-8.702	41.16	11.933	1.00	42.97
4605	CG2	THR	B	102	-7.062	39.723	10.895	1.00	42.76
4606	N	TYR	B	103	-4.306	40.145	12.889	1.00	37.13
4607	CA	TYR	B	103	-2.934	39.806	12.524	1.00	34.67
4608	C	TYR	B	103	-2.833	38.525	11.707	1.00	33.2
4609	O	TYR	B	103	-1.936	38.375	10.878	1.00	32.31
4610	CB	TYR	B	103	-2.057	39.709	13.774	1.00	34.15
4611	CG	TYR	B	103	-1.712	41.064	14.333	1.00	34.21
4612	CD1	TYR	B	103	-2.489	41.65	15.335	1.00	34.8
4613	CD2	TYR	B	103	-0.652	41.796	13.808	1.00	33.65
4614	CE1	TYR	B	103	-2.217	42.938	15.794	1.00	34.78
4615	CE2	TYR	B	103	-0.371	43.08	14.258	1.00	35.15
4616	CZ	TYR	B	103	-1.158	43.646	15.248	1.00	34.85
4617	OH	TYR	B	103	-0.897	44.927	15.666	1.00	36.01
4618	N	VAL	B	104	-3.758	37.606	11.949	1.00	31.83
4619	CA	VAL	B	104	-3.806	36.343	11.225	1.00	31.32
4620	C	VAL	B	104	-5.174	36.294	10.559	1.00	30.93
4621	O	VAL	B	104	-6.164	35.933	11.19	1.00	31.66
4622	CB	VAL	B	104	-3.662	35.143	12.18	1.00	31.77
4623	CG1	VAL	B	104	-3.649	33.844	11.388	1.00	31.54
4624	CG2	VAL	B	104	-2.39	35.289	13.002	1.00	31.49
4625	N	ASN	B	105	-5.228	36.662	9.284	1.00	29.88
4626	CA	ASN	B	105	-6.49	36.686	8.56	1.00	29.59
4627	C	ASN	B	105	-7.111	35.331	8.269	1.00	29.01
4628	O	ASN	B	105	-6.424	34.38	7.886	1.00	27.41
4629	CB	ASN	B	105	-6.338	37.443	7.235	1.00	29.54
4630	CG	ASN	B	105	-7.648	37.513	6.463	1.00	32.69
4631	OD1	ASN	B	105	-8.661	37.984	6.986	1.00	32.16
4632	ND2	ASN	B	105	-7.637	37.036	5.22	1.00	31.79
4633	N	THR	B	106	-8.424	35.256	8.461	1.00	30.12
4634	CA	THR	B	106	-9.177	34.041	8.175	1.00	31.7
4635	C	THR	B	106	-10.452	34.441	7.434	1.00	31.72
4636	O	THR	B	106	-11.385	33.65	7.305	1.00	31.97
4637	CB	THR	B	106	-9.557	33.266	9.456	1.00	32.45
4638	OG1	THR	B	106	-10.423	34.067	10.266	1.00	35.72
4639	CG2	THR	B	106	-8.306	32.896	10.25	1.00	33.62
4640	N	THR	B	107	-10.479	35.681	6.948	1.00	32.33

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

4641	CA	THR	B	107	-11.627	36.205	6.213	1.00	32.77
4642	C	THR	B	107	-11.39	36.059	4.711	1.00	32.61
4643	O	THR	B	107	-10.362	36.488	4.187	1.00	31.77
4644	CB	THR	B	107	-11.872	37.683	6.576	1.00	33.2
4645	OG1	THR	B	107	-12.204	37.767	7.967	1.00	34.43
4646	CG2	THR	B	107	-13.016	38.269	5.75	1.00	33.25
4647	N	LEU	B	108	-12.354	35.451	4.026	1.00	32.95
4648	CA	LEU	B	108	-12.245	35.193	2.593	1.00	33.2
4649	C	LEU	B	108	-11.936	36.384	1.682	1.00	33.82
4650	O	LEU	B	108	-10.957	36.353	0.927	1.00	33.25
4651	CB	LEU	B	108	-13.514	34.49	2.098	1.00	31.14
4652	CG	LEU	B	108	-13.844	33.165	2.796	1.00	32.02
4653	CD1	LEU	B	108	-15.088	32.549	2.172	1.00	30.87
4654	CD2	LEU	B	108	-12.657	32.204	2.68	1.00	30.44
4655	N	TYR	B	109	-12.764	37.423	1.756	1.00	34.11
4656	CA	TYR	B	109	-12.602	38.602	0.91	1.00	35.64
4657	C	TYR	B	109	-12.664	38.187	-0.559	1.00	36.01
4658	O	TYR	B	109	-13.613	37.531	-0.98	1.00	35.52
4659	CB	TYR	B	109	-11.273	39.319	1.189	1.00	36.7
4660	CG	TYR	B	109	-11.186	39.952	2.561	1.00	38.31
4661	CD1	TYR	B	109	-12.098	40.927	2.962	1.00	38.41
4662	CD2	TYR	B	109	-10.208	39.553	3.472	1.00	39.15
4663	CE1	TYR	B	109	-12.04	41.484	4.237	1.00	39.08
4664	CE2	TYR	B	109	-10.143	40.101	4.749	1.00	39.7
4665	CZ	TYR	B	109	-11.063	41.063	5.125	1.00	39.99
4666	OH	TYR	B	109	-11.019	41.573	6.4	1.00	41.27
4667	N	GLU	B	110	-11.647	38.562	-1.327	1.00	36.66
4668	CA	GLU	B	110	-11.598	38.244	-2.752	1.00	38.69
4669	C	GLU	B	110	-10.844	36.959	-3.068	1.00	37.46
4670	O	GLU	B	110	-11.051	36.36	-4.126	1.00	36.9
4671	CB	GLU	B	110	-10.942	39.393	-3.532	1.00	41.61
4672	CG	GLU	B	110	-11.691	40.718	-3.485	1.00	47.15
4673	CD	GLU	B	110	-13.087	40.621	-4.072	1.00	51
4674	OE1	GLU	B	110	-13.22	40.158	-5.228	1.00	53.63
4675	OE2	GLU	B	110	-14.053	41.01	-3.377	1.00	53.87
4676	N	LYS	B	111	-9.978	36.532	-2.154	1.00	35.87
4677	CA	LYS	B	111	-9.189	35.333	-2.39	1.00	34.83
4678	C	LYS	B	111	-8.501	34.812	-1.127	1.00	33.19
4679	O	LYS	B	111	-7.966	35.588	-0.336	1.00	32.8

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TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

4680	CB	LYS	B	111	-8.149	35.648	-3.474	1.00	36.38
4681	CG	LYS	B	111	-7.181	34.531	-3.821	1.00	38.88
4682	CD	LYS	B	111	-6.253	34.972	-4.948	1.00	40.46
4683	CE	LYS	B	111	-5.249	33.888	-5.323	1.00	42.9
4684	NZ	LYS	B	111	-4.397	34.288	-6.491	1.00	44.15
4685	N	PHE	B	112	-8.532	33.495	-0.938	1.00	31.35
4686	CA	PHE	B	112	-7.884	32.871	0.212	1.00	30.63
4687	C	PHE	B	112	-7.227	31.568	-0.225	1.00	30.05
4688	O	PHE	B	112	-7.807	30.791	-0.986	1.00	30.75
4689	CB	PHE	B	112	-8.879	32.578	1.335	1.00	29.49
4690	CG	PHE	B	112	-8.213	32.289	2.653	1.00	30.27
4691	CD1	PHE	B	112	-7.864	33.329	3.514	1.00	31.12
4692	CD2	PHE	B	112	-7.872	30.987	3.005	1.00	30.29
4693	CE1	PHE	B	112	-7.179	33.081	4.709	1.00	31.18
4694	CE2	PHE	B	112	-7.184	30.721	4.197	1.00	31.31
4695	CZ	PHE	B	112	-6.837	31.772	5.051	1.00	31.53
4696	N	THR	B	113	-6.023	31.321	0.274	1.00	28.72
4697	CA	THR	B	113	-5.288	30.124	-0.1	1.00	28.31
4698	C	THR	B	113	-4.845	29.271	1.086	1.00	28.43
4699	O	THR	B	113	-4.201	29.766	2.009	1.00	28.14
4700	CB	THR	B	113	-4.04	30.508	-0.912	1.00	28.89
4701	OG1	THR	B	113	-4.428	31.36	-2.001	1.00	28.7
4702	CG2	THR	B	113	-3.351	29.262	-1.458	1.00	27.71
4703	N	TYR	B	114	-5.201	27.988	1.06	1.00	27.27
4704	CA	TYR	B	114	-4.801	27.077	2.125	1.00	27.18
4705	C	TYR	B	114	-3.397	26.565	1.851	1.00	27.85
4706	O	TYR	B	114	-3.095	26.119	0.74	1.00	28.32
4707	CB	TYR	B	114	-5.732	25.868	2.22	1.00	25.73
4708	CG	TYR	B	114	-7.022	26.104	2.967	1.00	24.74
4709	CD1	TYR	B	114	-7.095	27.022	4.016	1.00	24.08
4710	CD2	TYR	B	114	-8.164	25.377	2.651	1.00	26.66
4711	CE1	TYR	B	114	-8.285	27.207	4.727	1.00	24.41
4712	CE2	TYR	B	114	-9.351	25.549	3.349	1.00	26.16
4713	CZ	TYR	B	114	-9.407	26.465	4.382	1.00	25.38
4714	OH	TYR	B	114	-10.597	26.644	5.036	1.00	24.73
4715	N	ALA	B	115	-2.542	26.627	2.866	1.00	27.29
4716	CA	ALA	B	115	-1.17	26.113	2.737	1.00	26.17
4717	C	ALA	B	115	-1.231	24.648	2.49	1.00	25.79
4718	O	ALA	B	115	-2.12	23.966	3.002	1.00	25



TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

4719	CB	ALA	B	115	-0.39	26.444	4.017	1.00	25.82
4720	N	GLY	B	116	-0.285	24.137	1.71	1.00	26.15
4721	CA	GLY	B	116	-0.268	22.719	1.406	1.00	28.15
4722	C	GLY	B	116	0.08	21.779	2.547	1.00	30.24
4723	O	GLY	B	116	0.814	22.13	3.479	1.00	28.41
4724	N	ILE	B	117	-0.463	20.57	2.465	1.00	32.41
4725	CA	ILE	B	117	-0.221	19.527	3.453	1.00	37.15
4726	C	ILE	B	117	0.371	18.33	2.715	1.00	41.64
4727	O	ILE	B	117	-0.326	17.657	1.952	1.00	41.47
4728	CB	ILE	B	117	-1.53	19.087	4.141	1.00	35.78
4729	CG1	ILE	B	117	-2.084	20.227	4.993	1.00	34.77
4730	CG2	ILE	B	117	-1.281	17.85	4.993	1.00	36.12
4731	CD1	ILE	B	117	-3.438	19.93	5.595	1.00	34.14
4732	N	ASP	B	118	1.658	18.073	2.93	1.00	46.97
4733	CA	ASP	B	118	2.322	16.953	2.269	1.00	52.65
4734	C	ASP	B	118	2.402	15.748	3.195	1.00	55.74
4735	O	ASP	B	118	3.185	15.739	4.148	1.00	56.29
4736	CB	ASP	B	118	3.737	17.336	1.83	1.00	53.85
4737	CG	ASP	B	118	4.409	16.236	1.024	1.00	56.01
4738	OD1	ASP	B	118	5.632	16.318	0.786	1.00	56.18
4739	OD2	ASP	B	118	3.705	15.285	0.622	1.00	57.29
4740	N	CYS	B	119	1.598	14.73	2.906	1.00	58.54
4741	CA	CYS	B	119	1.585	13.526	3.724	1.00	61.73
4742	C	CYS	B	119	2.783	12.629	3.428	1.00	62.67
4743	O	CYS	B	119	3.091	11.724	4.202	1.00	63.1
4744	CB	CYS	B	119	0.279	12.76	3.509	1.00	63.12
4745	SG	CYS	B	119	-1.197	13.718	3.959	1.00	66.66
4746	N	SER	B	120	3.457	12.884	2.31	1.00	64.05
4747	CA	SER	B	120	4.635	12.103	1.936	1.00	65.81
4748	C	SER	B	120	5.693	12.312	3.016	1.00	66.49
4749	O	SER	B	120	6.314	11.36	3.5	1.00	66.42
4750	CB	SER	B	120	5.185	12.572	0.585	1.00	66.12
4751	OG	SER	B	120	4.204	12.468	-0.432	1.00	66.9
4752	N	ALA	B	121	5.888	13.575	3.38	1.00	66.86
4753	CA	ALA	B	121	6.844	13.954	4.411	1.00	67.46
4754	C	ALA	B	121	6.066	14.095	5.71	1.00	67.67
4755	O	ALA	B	121	6.206	15.085	6.428	1.00	68.47
4756	CB	ALA	B	121	7.505	15.281	4.048	1.00	67.25
4757	N	GLU	B	122	5.242	13.095	6.004	1.00	67.58

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

4758	CA	GLU	B	122	4.42	13.116	7.205	1.00	67.46
4759	C	GLU	B	122	3.696	11.781	7.384	1.00	68.09
4760	O	GLU	B	122	2.446	11.762	7.351	1.00	68.87
4761	CB	GLU	B	122	3.418	14.271	7.098	1.00	66.2
4762	CG	GLU	B	122	2.445	14.4	8.248	1.00	64.52
4763	CD	GLU	B	122	1.575	15.632	8.121	1.00	62.9
4764	OE1	GLU	B	122	0.57	15.721	8.852	1.00	63.35
4765	OE2	GLU	B	122	1.9	16.514	7.301	1.00	60.82
4766	OXT	GLU	B	122	4.394	10.758	7.551	1.00	68.5
4767	O	HOH		1	17.842	-24.632	17.33	1.00	21.58
4768	O	HOH		2	19.03	-22.853	15.79	1.00	20.98
4769	O	HOH		3	10.397	-19.402	24.693	1.00	25.64
4770	O	HOH		4	12.125	-17.225	25.143	1.00	31.09
4771	O	HOH		5	8.501	-22.109	14.394	1.00	20.44
4772	O	HOH		6	9.555	-22.226	10.96	1.00	25.21
4773	O	HOH		7	3.403	19.443	13.901	1.00	18.33
4774	O	HOH		8	-7.281	15.668	32.833	1.00	22.19
4775	O	HOH		9	16.44	-35.885	37.402	1.00	33.52
4776	O	HOH		10	18.132	-33.584	36.916	1.00	33.31
4777	O	HOH		11	17.424	-31.882	35.008	1.00	23.59
4778	O	HOH		12	2.576	-25.457	4.306	1.00	21.04
4779	O	HOH		13	12.104	22.068	19.994	1.00	21.41
4780	O	HOH		14	15.46	22.378	20.477	1.00	26.54
4781	O	HOH		15	-1.377	13.183	19.622	1.00	17.01
4782	O	HOH		16	0.408	14.413	17.905	1.00	30.15
4783	O	HOH		17	-8.863	-2.086	35.98	1.00	35.26
4784	O	HOH		18	3.225	-13.115	26.556	1.00	19.29
4785	O	HOH		19	-11.258	-15.785	27.114	1.00	21.05
4786	O	HOH		20	5.534	-14.247	25.544	1.00	30.94
4787	O	HOH		21	3.865	-22.233	37.641	1.00	27.07
4788	O	HOH		22	21.071	-26.279	29.424	1.00	29.67
4789	O	HOH		23	19.483	-24.208	29.705	1.00	24.67
4790	O	HOH		24	22.647	-25.562	32.013	1.00	43.28
4791	O	HOH		25	21.981	-26.133	26.326	1.00	33.76
4792	O	HOH		26	15.739	-27.899	34.558	1.00	22.62
4793	O	HOH		27	16.124	-30.295	33.119	1.00	26.79
4794	O	HOH		28	20.779	-34.199	38.16	1.00	35.3
4795	O	HOH		29	24.528	-31.621	37.868	1.00	37.08
4796	O	HOH		30	16.318	-36.545	40.442	1.00	31.36

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

4797	O	HOH		31	16.908	-38.267	36.231	1.00	51.96
4798	O	HOH		32	4.872	-39.475	32.466	1.00	33.29
4799	O	HOH		33	3.128	-38.039	36.077	1.00	32.56
4800	O	HOH		34	-1.039	-42.707	20.019	1.00	31.82
4801	O	HOH		35	-3.265	-39.314	17.586	1.00	40.19
4802	O	HOH		36	-5.025	-36.398	21.078	1.00	30.14
4803	O	HOH		37	4.512	-41.461	15.035	1.00	39.34
4804	O	HOH		38	0.411	-33.438	10.694	1.00	21.38
4805	O	HOH		39	2.804	-31.935	10.094	1.00	41.73
4806	O	HOH		40	10.863	-28.524	3.662	1.00	33.63
4807	O	HOH		41	20.498	-35.286	10.565	1.00	28.65
4808	O	HOH		42	22.939	-30.663	10.468	1.00	37.53
4809	O	HOH		43	18.918	-34.316	15.591	1.00	31.32
4810	O	HOH		44	19.43	-40.59	24.823	1.00	35.43
4811	O	HOH		45	16.012	-43.124	29.438	1.00	37.83
4812	O	HOH		46	19.445	-28.881	18.613	1.00	23.27
4813	O	HOH		47	13.707	-21.082	27.141	1.00	19.77
4814	O	HOH		48	14.69	-18.548	26.267	1.00	31.42
4815	O	HOH		49	11.03	-21.263	13.156	1.00	35.5
4816	O	HOH		50	13.004	-22.336	11.755	1.00	22.5
4817	O	HOH		51	3.312	-25.427	10.052	1.00	22.24
4818	O	HOH		52	5.087	-25.789	4.405	1.00	28.08
4819	O	HOH		53	11.979	-26.584	5.348	1.00	37.16
4820	O	HOH		54	14.355	-14.663	9.03	1.00	38.69
4821	O	HOH		55	-0.484	-12.664	9.251	1.00	33.01
4822	O	HOH		56	-2.395	-12.369	11.253	1.00	37.24
4823	O	HOH		57	-8.268	-19.596	27.674	1.00	28.76
4824	O	HOH		58	-10.735	-19.852	26.722	1.00	26.4
4825	O	HOH		59	-9.604	-24.355	27.812	1.00	48.62
4826	O	HOH		60	6.218	-13.698	21.328	1.00	26.05
4827	O	HOH		61	4.931	-15.734	15.039	1.00	39.49
4828	O	HOH		62	1.619	-25.884	6.828	1.00	42.77
4829	O	HOH		63	-4.977	-31.913	15.559	1.00	34.25
4830	O	HOH		64	-2.866	-32.853	26.043	1.00	34.52
4831	O	HOH		65	-0.913	-29.919	31.429	1.00	28.91
4832	O	HOH		66	-3.009	-31.895	32.394	1.00	50.39
4833	O	HOH		67	-4.574	-31.498	29.818	1.00	47.72
4834	O	HOH		68	6.041	-36.462	37.939	1.00	41.3
4835	O	HOH		69	1.308	-31.948	39.631	1.00	55.97

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TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

4836	O	HOH		70	6.077	-32.991	40.238	1.00	36.23
4837	O	HOH		71	8.587	-36.723	50.124	1.00	43.53
4838	O	HOH		72	2.409	24.312	3.694	1.00	23.86
4839	O	HOH		73	3.289	26.332	2.104	1.00	40.12
4840	O	HOH		74	1.677	25.587	-0.205	1.00	35.76
4841	O	HOH		75	6.38	26.067	2.959	1.00	31.16
4842	O	HOH		76	-3.531	27.965	5.211	1.00	22.53
4843	O	HOH		77	-1.944	30.283	5.411	1.00	25.58
4844	O	HOH		78	0.142	30.638	3.338	1.00	30.65
4845	O	HOH		79	-3.174	31.816	3.449	1.00	23.69
4846	O	HOH		80	-4.898	33.646	1.794	1.00	30.18
4847	O	HOH		81	-4.623	34.16	-0.928	1.00	33.69
4848	O	HOH		82	-8.653	36.522	2.21	1.00	28.78
4849	O	HOH		83	-5.829	36.103	3.381	1.00	34.64
4850	O	HOH		84	-4.153	38.669	3.21	1.00	54.29
4851	O	HOH		85	-5.77	39.258	16.051	1.00	28.97
4852	O	HOH		86	-10.005	37.99	16.009	1.00	28.9
4853	O	HOH		87	-9.347	43.689	21.112	1.00	45.94
4854	O	HOH		88	3.033	42.689	26.449	1.00	28.12
4855	O	HOH		89	2.626	41.133	28.609	1.00	42.98
4856	O	HCH		90	4.099	39.142	29.56	1.00	36.25
4857	O	HOH		91	6.758	37.795	28.883	1.00	35.75
4858	O	HOH		92	0.458	36.189	29.604	1.00	33.53
4859	O	HOH		93	9.665	41.472	23.441	1.00	29.58
4860	O	HOH		94	10.289	40.059	28.175	1.00	34.27
4861	O	HOH		95	11.954	33.439	28.768	1.00	23.28
4862	O	HOH		96	13.677	35.314	30.128	1.00	42.99
4863	O	HOH		97	14.017	37.56	28.644	1.00	42.66
4864	O	HOH		98	5.699	31.977	31.719	1.00	24.42
4865	O	HOH		99	13.646	31.335	26.726	1.00	50.06
4866	O	HOH		100	20.167	35.38	10.434	1.00	32.67
4867	O	HOH		101	17.856	35.066	8.874	1.00	44.77
4868	O	HOH		102	15.041	34.525	9.852	1.00	30.19
4869	O	HOH		103	16.544	37.9	9.615	1.00	55.02
4870	O	HOH		104	15.395	39.384	12.07	1.00	53.77
4871	O	HOH		105	1.273	43.179	6.997	1.00	37.75
4872	O	HOH		106	8.436	35.916	2.292	1.00	35.62
4873	O	HOH		107	7.775	28.44	2.668	1.00	39.84
4874	O	HOH		108	9.116	26.703	1.207	1.00	38.19

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TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

4875	O	HOH		109	12.476	29.084	8.224	1.00	22.54
4876	O	HOH		110	2.569	20.931	10.083	1.00	28.18
4877	O	HOH		111	3.775	18.52	9.489	1.00	35.72
4878	O	HOH		112	3.904	17.222	12.367	1.00	28.28
4879	O	HOH		113	13.782	25.461	26.446	1.00	21.4
4880	O	HOH		114	19.735	25.778	26.976	1.00	26.77
4881	O	HOH		115	18.702	25.432	29.499	1.00	29.23
4882	O	HOH		116	19.22	14.933	16.642	1.00	40.7
4883	O	HOH		117	16.249	22.281	17.028	1.00	23.43
4884	O	HOH		118	13.937	21.442	18.184	1.00	41.23
4885	O	HOH		119	15.006	22.992	9.868	1.00	15.99
4886	O	HOH		120	12.999	24.651	10.25	1.00	24.9
4887	O	HOH		121	22.679	26.517	31.783	1.00	29.04
4888	O	HOH		122	13.053	12.584	30.194	1.00	30.27
4889	O	HOH		123	10.788	12.526	31.28	1.00	32.53
4890	O	HOH		124	-6.103	28.916	23.973	1.00	35.85
4891	O	HOH		125	-7.271	30.136	21.634	1.00	27.46
4892	O	HOH		126	-9.001	31.513	22.814	1.00	42.78
4893	O	HOH		127	-11.188	30.021	22.764	1.00	39.52
4894	O	HOH		128	-7.631	24.113	31.102	1.00	47.54
4895	O	HOH		129	-7.216	19.659	29.615	1.00	22.23
4896	O	HOH		130	-9.631	17.16	31.059	1.00	50.41
4897	O	HOH		131	4.791	13.688	18.904	1.00	29.73
4898	O	HOH		132	8.63	13.987	20.203	1.00	40.63
4899	O	HOH		133	2.086	14.862	12.599	1.00	37.52
4900	O	HOH		134	15.664	14.721	20.484	1.00	49.49
4901	O	HOH		135	3.894	31.735	33.351	1.00	31.19
4902	O	HOH		136	-3.508	32.994	25.721	1.00	43.49
4903	O	HOH		137	-10.676	36.834	12.694	1.00	38.53
4904	O	HOH		138	-11	22.337	14.697	1.00	29.42
4905	O	HOH		139	-13.003	23.883	15.802	1.00	53.22
4906	O	HOH		140	-5.551	13.541	25.991	1.00	30.54
4907	O	HOH		141	-0.802	24.985	37.276	1.00	48.41
4908	O	HOH		142	5.163	24.722	40.085	1.00	37
4909	O	HOH		143	6.091	17.632	38.542	1.00	53.22
4910	O	HOH		144	0.732	3.799	27.764	1.00	40
4911	O	HOH		145	3.962	5.01	22.596	1.00	35.92
4912	O	HOH		146	1.19	10.78	19.952	1.00	47.33
4913	O	HOH		147	-14.74	1.831	26.894	1.00	31.84

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TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

4914	O	HOH		148	-13.895	0.285	29.919	1.00	45.97
4915	O	HOH		149	-11.095	-0.388	33.819	1.00	46.61
4916	O	HOH		150	-7.043	6.856	43.959	1.00	35.08
4917	O	HOH		151	-21.246	-6.659	21.926	1.00	36.2
4918	O	HOH		152	-19.328	-7.8	23.425	1.00	51.79
4919	O	HOH		153	7.91	-35.169	41.66	1.00	45.67
4920	O	HOH		154	4.786	-35.935	40.356	1.00	46.94
4921	O	HOH		155	13.729	-39.766	33.293	1.00	36.27
4922	O	HOH		156	3.492	-41.405	31.076	1.00	27.62
4923	O	HOH		157	4.309	-40.11	34.996	1.00	38.34
4924	O	HOH		158	8.587	-44.603	35.954	1.00	35.18
4925	O	HOH		159	1.748	-48.877	31.706	1.00	40.57
4926	O	HOH		160	-2.599	-43.491	22.685	1.00	45.37
4927	O	HOH		161	-0.862	-46.242	22.479	1.00	45.67
4928	O	HOH		162	-3.158	-41.731	19.015	1.00	52.69
4929	O	HOH		163	-1.992	-37.835	15.458	1.00	29.41
4930	O	HOH		164	-2.087	-39.886	13.31	1.00	36.58
4931	O	HOH		165	0.601	-40.15	12.651	1.00	32.9
4932	O	HOH		166	0.652	-39.816	9.931	1.00	33.1
4933	O	HOH		167	1.679	-37.74	9.014	1.00	31.67
4934	O	HOH		168	-0.161	-35.192	8.685	1.00	38.23
4935	O	HOH		169	2.496	-42.223	13.3	1.00	30.27
4936	O	HOH		170	3.552	-42.884	11.226	1.00	38.85
4937	O	HOH		171	7.737	-40.994	13.66	1.00	39.15
4938	O	HOH		172	8.708	-38.155	7.445	1.00	72.84
4939	O	HOH		173	8.993	-39.911	10.807	1.00	52.2
4940	O	HOH		174	8.243	-32.591	3.423	1.00	47.08
4941	O	HOH		175	12.433	-30.257	2.179	1.00	56.37
4942	O	HOH		176	8.296	-27.759	2.395	1.00	47.45
4943	O	HOH		177	18.477	-38.587	10.307	1.00	47.39
4944	O	HOH		178	20.934	-35.079	13.713	1.00	44.06
4945	O	HOH		179	16.766	-39.727	14.522	1.00	50.87
4946	O	HOH		180	10.818	-41.433	20.399	1.00	54.45
4947	O	HOH		181	22.595	-38.362	24.674	1.00	52.87
4948	O	HOH		182	22.988	-35.512	25.128	1.00	39.38
4949	O	HOH		183	22.687	-28.507	25.593	1.00	37.98
4950	O	HOH		184	25.439	-32.555	19.99	1.00	54.33
4951	O	HOH		185	24.979	-16.318	25.447	1.00	54.24
4952	O	HOH		186	19.295	-15.203	4.185	1.00	51.28

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TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

4953	O	HOH		187	0.366	-15.464	4.448	1.00	30.61
4954	O	HOH		188	2.756	-14.805	4.194	1.00	33.75
4955	O	HOH		189	-2.067	-15.165	11.979	1.00	31.53
4956	O	HOH		190	-7.663	-22.151	34.838	1.00	42.59
4957	O	HOH		191	-10.4	-17.146	29.532	1.00	41.64
4958	O	HOH		192	8.282	-14.619	28.589	1.00	57.27
4959	O	HOH		193	11.278	-14.985	26.305	1.00	39.66
4960	O	HOH		194	10.766	-19.456	17.66	1.00	40.6
4961	O	HOH		195	6.693	-13.978	16.822	1.00	46.42
4962	O	HOH		196	6.414	-11.324	19.655	1.00	56.51
4963	O	HOH		197	11.15	-15.456	12.846	1.00	49.5
4964	O	HOH		198	9.377	-14.875	10.818	1.00	45.26
4965	O	HOH		199	3.907	-13.483	14.421	1.00	34.66
4966	O	HOH		200	1.607	-30.11	5.988	1.00	51.93
4967	O	HOH		201	-6.306	-31.283	11.598	1.00	46.89
4968	O	HOH		202	-7.613	-31.254	13.987	1.00	39.75
4969	O	HOH		203	-12.634	-24.887	12.368	1.00	31.94
4970	O	HOH		204	-5.261	-30.946	27.056	1.00	50.02
4971	O	HOH		205	0.674	-37.887	37.463	1.00	40.19
4972	O	HOH		206	-0.343	-34.929	37.299	1.00	38.47
4973	O	HOH		207	1.676	-35.991	41.395	1.00	51.91
4974	O	HOH		208	-0.051	-28.45	39.068	1.00	48.77
4975	O	HOH		209	2.181	-24.152	38.897	1.00	49.77
4976	O	HOH		210	10.891	-28.946	54.419	1.00	49.8
4977	O	HOH		211	6.597	-23.781	52.454	1.00	53.54
4978	O	HOH		212	3.678	-24.11	46.592	1.00	50.53
4979	O	HOH		213	16.479	-22.304	46.221	1.00	45.15
4980	O	HOH		214	5.989	-19.352	41.498	1.00	40.3
4981	O	HOH		215	9.406	-16.226	34.783	1.00	43.61
4982	O	HOH		216	2.733	-17.756	34.487	1.00	48.41
4983	O	HOH		217	-1.258	-18.577	37.075	1.00	39.97
4984	O	HOH		218	-4.608	-18.985	39.025	1.00	62.88
4985	O	HOH		219	-4.835	6.492	18.253	1.00	51.83
4986	O	HOH		220	-3.542	-3.838	21.448	1.00	26.04
4987	O	HOH		221	-14.764	-15.794	31.351	1.00	41.53
4988	O	HOH		222	2.548	-5.031	20.882	1.00	39.88
4989	O	HOH		223	1.812	-9.857	30.651	1.00	40.67
4990	O	HOH		224	-16.166	0.071	25.807	1.00	35.51
4991	O	HOH		225	-18.459	2.24	26.604	1.00	53.53

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TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

4992	O	HOH		226	-19.783	-2.756	16.555	1.00	38.18
4993	O	HOH		227	-17.993	-2.662	14.593	1.00	44.05
4994	O	HOH		228	-1.258	29.652	1.609	1.00	41.29
4995	O	HOH		229	2.202	28.908	2.996	1.00	49.11
4996	O	HOH		230	-13.525	35.446	9.25	1.00	41.86
4997	O	HOH		231	-5.308	41.469	17.89	1.00	30.96
4998	O	HOH		232	8.759	39.997	30.238	1.00	31.49
4999	O	HOH		233	12.759	39.66	29.325	1.00	43.66
5000	O	HOH		234	10.481	42.159	25.998	1.00	34.85
5001	O	HOH		235	21.695	32.722	24.562	1.00	41.04
5002	O	HOH		236	27.737	38.273	17.432	1.00	53.74
5003	O	HOH		237	22.826	28.792	22.069	1.00	45.31
5004	O	HOH		238	25.051	30.055	21.018	1.00	44.78
5005	O	HOH		239	21.717	26.575	20.567	1.00	36.09
5006	O	HOH		240	22.014	36.251	13.667	1.00	34.29
5007	O	HOH		241	19.597	38.697	11.408	1.00	62.9
5008	O	HOH		242	6.898	40.697	5.643	1.00	36.19
5009	O	HOH		243	8.595	41.455	8.661	1.00	51.81
5010	O	HOH		244	-2.12	39.573	5.41	1.00	48.43
5011	O	HOH		245	-3.249	39.937	7.75	1.00	40.27
5012	O	HOH		246	7.666	38.414	2.784	1.00	49.93
5013	O	HOH		247	15.895	34.561	3.789	1.00	47.13
5014	O	HOH		248	25.619	25.63	12.797	1.00	45.65
5015	O	HOH		249	17.887	15.405	31.176	1.00	33.21
5016	O	HOH		250	9.801	15.174	30.322	1.00	22.88
5017	O	HOH		251	10.427	13.701	24.258	1.00	32.85
5018	O	HOH		252	9.748	15.98	22.858	1.00	42.4
5019	O	HOH		253	11.283	10.795	24.156	1.00	61.93
5020	O	HOH		254	-3.965	29.559	29.96	1.00	42.21
5021	O	HOH		255	-5.153	30.347	27.617	1.00	38.87
5022	O	HOH		256	-3.099	31.405	31.574	1.00	42.53
5023	O	HOH		257	-0.28	14.934	14.505	1.00	41.34
5024	O	HOH		258	11.543	29.33	37.169	1.00	38.87
5025	O	HOH		259	9.538	28.802	35.559	1.00	26.84
5026	O	HOH		260	5.27	31.179	35.467	1.00	36.74
5027	O	HOH		261	-4.924	33.232	28.072	1.00	38.32
5028	O	HOH		262	-8.459	38.488	23.829	1.00	49.12
5029	O	HOH		263	-23.446	29.205	1.777	1.00	56.19
5030	O	HOH		264	-12.934	18.711	19.598	1.00	36.31



TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

5031	O	HOH		265	-12.467	20.493	15.734	1.00	41.22
5032	O	HOH		266	-14.002	15.289	23.167	1.00	53.75
5033	O	HOH		267	-10.401	10.65	23.427	1.00	53.87
5034	O	HOH		268	-1.141	-1.488	42.339	1.00	51.47
5035	O	HOH		269	-2.892	0.32	43.835	1.00	35.25
5036	O	HOH		270	0.922	2.473	43.95	1.00	53.53
5037	O	HOH		271	-16.794	12.745	41.117	1.00	46.97
5038	O	HOH		272	-17.385	8.214	37.926	1.00	44.44
5039	O	HOH		273	-15.476	6.385	36.581	1.00	38.39
5040	O	HOH		274	-8.916	11.275	46.327	1.00	43.8
5041	O	HOH		275	-5.666	12.989	45.457	1.00	41.79
5042	O	HOH		276	-11.357	10.166	30.033	1.00	43.78
5043	O	HOH		277	-13.813	6.8	25.4	1.00	43.3
5044	O	HOH		278	-5.616	9.906	19.335	1.00	39.83
5045	O	HOH		279	-3.996	13.495	19.575	1.00	42.56
5046	O	HOH		280	-16.429	-7.499	13.456	1.00	34.05
5047	O	HOH		281	-19.688	-0.483	18.276	1.00	31.93
5048	O	HOH		282	-17.712	1.029	17.53	1.00	40.33
5049	O	HOH		283	-25.514	-5.566	26.454	1.00	46.07
5050	O	HOH		284	-10.361	-10.194	31.94	1.00	44.55
5051	O	HCH		285	-4.26	-13.425	27.79	1.00	28.14
5052	O	HOH		286	1.902	-13.554	29.317	1.00	43.54
5053	O	HOH		287	3.857	-10.723	24.158	1.00	32.9
5054	O	HOH		288	4.033	-10.717	15.203	1.00	38.95
5055	O	HOH		289	2.464	-7.689	17.421	1.00	38.1
5056	O	HOH		290	1.315	-5.608	16.053	1.00	45.37
5057	O	HOH		291	-1.687	-3.203	19.185	1.00	50.35
5058	O	HOH		292	-2.396	-1.624	23.064	1.00	42.61
5059	O	HOH		293	0.899	-1.226	24.966	1.00	41.61
5060	O	HOH		294	-17.824	-6.882	33.396	1.00	32.63
5061	O	HOH		295	-24.32	-11.426	23.056	1.00	41.33
5062	O	HOH		296	-22.424	-13.176	21.03	1.00	37.55
5063	O	HOH		297	-1.79	-1.764	14.721	1.00	46.75
5064	O	HOH		298	-1.847	-4.586	14.478	1.00	52.15
5065	O	HOH		299	-10.955	-17.318	12.812	1.00	44.43
5066	O	HOH		300	-14.069	-19.916	20.346	1.00	44.59
5067	O	HOH		301	-13.24	-19.883	23.691	1.00	38.35
5068	O	HOH		302	-12.311	-24.293	20.066	1.00	38.3
5069	O	HOH		303	2.2	-20.402	38.413	1.00	33.32

TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

5070	O	HOH		304	3.499	-19.098	40.465	1.00	44.82
5071	O	HOH		305	8.028	-17.205	40.838	1.00	41.72
5072	O	HOH		306	10.497	-16.859	37.311	1.00	42.16
5073	O	HOH		307	10.551	-22.274	51.41	1.00	41.15
5074	O	HOH		308	4.129	-31.425	43.018	1.00	41.45
5075	O	HOH		309	3.338	-32.944	41.121	1.00	41.58
5076	O	HOH		310	0.185	-26.465	37.638	1.00	47.07
5077	O	HOH		311	-3.309	-29.998	34.586	1.00	42.31
5078	O	HOH		312	-2.724	-29.094	29.312	1.00	31.54
5079	O	HOH		313	-4.07	-36.748	25.411	1.00	47.05
5080	O	HOH		314	-6.711	-28.541	10.227	1.00	32.04
5081	O	HOH		315	-7.282	-33.363	10.089	1.00	40.93
5082	O	HOH		316	-10.088	-29.765	11.981	1.00	50.87
5083	O	HOH		317	3.126	-11.219	9.3	1.00	51.11
5084	O	HOH		318	24.229	-26.438	24.448	1.00	45.74
5085	O	HOH		319	18.975	-30.694	32.165	1.00	35.88
5086	O	HOH		320	18.97	-39.786	18.415	1.00	41.98
5087	O	HOH		321	7.531	-39.219	15.988	1.00	30.93
5088	O	HOH		322	18.786	-35.829	8.028	1.00	35.9
5089	O	HOH		323	8.513	-34.064	6.734	1.00	37.31
5090	O	HOH		324	3.219	-37.701	6.726	1.00	43.31
5091	O	HOH		325	5.507	-46.232	20.109	1.00	43.77
5092	O	HOH		326	6.858	-48.369	28.595	1.00	40.12
5093	O	HOH		327	5.981	-43.678	37.125	1.00	38.67
5094	O	HOH		328	10.537	-40.326	38.412	1.00	39.32
5095	O	HOH		329	13.175	-38.597	46.111	1.00	48.54
5096	O	HOH		330	-7.204	6.769	41.203	1.00	39.55
5097	O	HOH		331	-6.552	13.802	23.556	1.00	39.72
5098	O	HOH		332	0.39	1.348	26.59	1.00	42.24
5099	O	HOH		333	3.784	3.049	26.657	1.00	53.59
5100	O	HOH		334	3.366	0.297	28.177	1.00	40.66
5101	O	HOH		335	7.8	4.615	28.788	1.00	42.86
5102	O	HOH		336	2.999	27.7	37.623	1.00	35.96
5103	O	HOH		337	5.649	29.765	37.748	1.00	45.48
5104	O	HOH		338	8.45	29.127	38.021	1.00	44.26
5105	O	HOH		339	-3.421	15.2	10.661	1.00	54
5106	O	HOH		340	-2.988	14.951	13.445	1.00	45.28
5107	O	HOH		341	-13.823	18.956	13.808	1.00	40.97
5108	O	HOH		342	-20.773	22.637	3.033	1.00	48.96

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TABLE 2  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM 1

5109	O	HOH		343	-9.909	34.773	21.545	1.00	40.68
5110	O	HOH		344	-12.731	34.894	18.707	1.00	41.56
5111	O	HOH		345	-12.061	37.704	17.37	1.00	37.67
5112	O	HOH		346	8.457	31.431	34.824	1.00	50.77
5113	O	HOH		347	9.4	33.136	36.349	1.00	47.68
5114	O	HOH		348	14.066	16.238	18.043	1.00	41.55
5115	O	HOH		349	10.161	19.473	16.513	1.00	37.38
5116	O	HOH		350	-13.303	22.596	26.206	1.00	40.02
5117	O	HOH		351	-5.801	28.694	31.776	1.00	32.49
5118	O	HOH		352	24.539	26.298	20.343	1.00	48.73
5119	O	HOH		353	26.084	25.668	18.379	1.00	44.38
5120	O	HOH		354	26.126	13.685	15.048	1.00	41.24
5121	O	HOH		355	2.768	36.754	1.668	1.00	36.05
5122	O	HOH		356	21.668	30.916	8.242	1.00	42.96
5123	O	HOH		357	10.186	39.262	20.246	1.00	36.1
5124	O	HOH		358	12.137	40.996	21.542	1.00	44.58
5125	O	HOH		359	-10.126	37.578	9.889	1.00	39.65
5126	O	HOH		360	-9.779	40.084	8.38	1.00	40.17
5127	O	HOH		361	7.135	18.022	1.084	1.00	41.63

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

ATOM	ATOM TYPE	RESIDUE	PROTEIN #	#	X	Y	Z	OCC	B
1	N	PRO	A	813	-14.726	7.43	13.296	1.00	61.71
2	CA	PRO	A	813	-15.304	8.732	13.717	1.00	61.69
3	C	PRO	A	813	-16.201	8.547	14.941	1.00	61.37
4	O	PRO	A	813	-17.251	7.909	14.853	1.00	60.99
5	CB	PRO	A	813	-16.108	9.265	12.537	1.00	62.02
6	CG	PRO	A	813	-15.44	8.55	11.361	1.00	61.83
7	CD	PRO	A	813	-15.102	7.147	11.9	1.00	61.79
8	N	THR	A	814	-15.792	9.111	16.076	1.00	60.62
9	CA	THR	A	814	-16.563	8.986	17.31	1.00	59.24
10	C	THR	A	814	-17.448	10.199	17.598	1.00	59.08
11	O	THR	A	814	-17.046	11.345	17.395	1.00	58.6
12	CB	THR	A	814	-15.642	8.777	18.529	1.00	59.26
13	OG1	THR	A	814	-14.639	7.805	18.211	1.00	60.37
14	CG2	THR	A	814	-16.452	8.285	19.728	1.00	57.66
15	N	ILE	A	815	-18.657	9.93	18.078	1.00	58.24
16	CA	ILE	A	815	-19.604	10.983	18.415	1.00	57.11
17	C	ILE	A	815	-19.917	10.92	19.917	1.00	55.96
18	O	ILE	A	815	-20.71	10.093	20.375	1.00	55.8
19	CB	ILE	A	815	-20.898	10.848	17.559	1.00	57.13
20	CG1	ILE	A	815	-22.042	11.634	18.197	1.00	57.59
21	CG2	ILE	A	815	-21.25	9.389	17.368	1.00	57.92
22	CD1	ILE	A	815	-21.802	13.123	18.256	1.00	59.9
23	N	TYR	A	816	-19.266	11.797	20.677	1.00	53.87
24	CA	TYR	A	816	-19.431	11.854	22.125	1.00	51.96
25	C	TYR	A	816	-20.535	12.84	22.493	1.00	48.69
26	O	TYR	A	816	-20.96	13.641	21.663	1.00	48.81
27	CB	TYR	A	816	-18.116	12.286	22.791	1.00	54.23
28	CG	TYR	A	816	-16.887	12.023	21.952	1.00	55.94
29	CD1	TYR	A	816	-16.619	12.794	20.819	1.00	56.88
30	CD2	TYR	A	816	-16.015	10.978	22.261	1.00	56.64
31	CE1	TYR	A	816	-15.52	12.529	20.009	1.00	58
32	CE2	TYR	A	816	-14.907	10.704	21.455	1.00	57.62
33	CZ	TYR	A	816	-14.67	11.484	20.329	1.00	58.02
34	OH	TYR	A	816	-13.6	11.21	19.508	1.00	58.98
35	N	PRO	A	817	-21.005	12.8	23.751	1.00	45.58
36	CA	PRO	A	817	-20.552	11.889	24.808	1.00	44.23
37	C	PRO	A	817	-20.91	10.419	24.579	1.00	43.38
38	O	PRO	A	817	-21.962	10.098	24.018	1.00	42.45
39	CB	PRO	A	817	-21.216	12.464	26.06	1.00	44.46

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

40	CG	PRO	A	817	-22.487	13.038	25.53	1.00	44.2
41	CD	PRO	A	817	-22.027	13.73	24.267	1.00	44.54
42	N	VAL	A	818	-20.018	9.533	25.012	1.00	42.51
43	CA	VAL	A	818	-20.229	8.096	24.88	1.00	42.17
44	C	VAL	A	818	-21.253	7.675	25.92	1.00	42.75
45	O	VAL	A	818	-20.999	7.761	27.12	1.00	44.28
46	CB	VAL	A	818	-18.919	7.311	25.119	1.00	41.77
47	CG1	VAL	A	818	-19.203	5.817	25.191	1.00	40.3
48	CG2	VAL	A	818	-17.931	7.611	24.001	1.00	41.57
49	N	LEU	A	819	-22.414	7.23	25.461	1.00	42.55
50	CA	LEU	A	819	-23.468	6.817	26.372	1.00	42.7
51	C	LEU	A	819	-23.329	5.345	26.732	1.00	43.13
52	O	LEU	A	819	-22.825	4.543	25.943	1.00	42.35
53	CB	LEU	A	819	-24.831	7.064	25.733	1.00	43.24
54	CG	LEU	A	819	-25.033	8.451	25.12	1.00	42.89
55	CD1	LEU	A	819	-26.28	8.446	24.257	1.00	43.07
56	CD2	LEU	A	819	-25.132	9.492	26.219	1.00	42.69
57	N	ASP	A	820	-23.775	5.001	27.935	1.00	43.52
58	CA	ASP	A	820	-23.72	3.627	28.417	1.00	43.1
59	C	ASP	A	820	-25.056	2.946	28.118	1.00	41.42
60	O	ASP	A	820	-26.102	3.371	28.608	1.00	40.64
61	CB	ASP	A	820	-23.426	3.621	29.921	1.00	46.04
62	CG	ASP	A	820	-23.42	2.225	30.508	1.00	49.67
63	OD1	ASP	A	820	-22.834	1.314	29.88	1.00	52.26
64	OD2	ASP	A	820	-23.991	2.043	31.606	1.00	50.56
65	N	TRP	A	821	-25.006	1.891	27.308	1.00	39.62
66	CA	TRP	A	821	-26.201	1.155	26.901	1.00	37.23
67	C	TRP	A	821	-27.18	0.825	28.016	1.00	35.9
68	O	TRP	A	821	-28.387	0.809	27.794	1.00	36.24
69	CB	TRP	A	821	-25.798	-0.129	26.165	1.00	37.34
70	CG	TRP	A	821	-26.945	-1.067	25.888	1.00	37
71	CD1	TRP	A	821	-27.425	-2.049	26.714	1.00	36.27
72	CD2	TRP	A	821	-27.783	-1.078	24.725	1.00	35.62
73	NE1	TRP	A	821	-28.51	-2.668	26.137	1.00	36.01
74	CE2	TRP	A	821	-28.752	-2.092	24.917	1.00	35.54
75	CE3	TRP	A	821	-27.812	-0.33	23.541	1.00	34.72
76	CZ2	TRP	A	821	-29.74	-2.374	23.967	1.00	33.87
77	CZ3	TRP	A	821	-28.796	-0.611	22.597	1.00	34.39
78	CH2	TRP	A	821	-29.747	-1.626	22.818	1.00	34.06
79	N	ASN	A	822	-26.672	0.561	29.213	1.00	35.21

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TABLE 3

STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

80	CA	ASN	A	822	-27.548	0.23	30.328	1.00	35.75
81	C	ASN	A	822	-28.338	1.424	30.823	1.00	35.52
82	O	ASN	A	822	-29.366	1.26	31.475	1.00	35.75
83	CB	ASN	A	822	-26.745	-0.366	31.477	1.00	38.29
84	CG	ASN	A	822	-26.277	-1.772	31.182	1.00	40.64
85	OD1	ASN	A	822	-27.089	-2.695	31.075	1.00	42.19
86	ND2	ASN	A	822	-24.963	-1.946	31.037	1.00	40.18
87	N	ASP	A	823	-27.856	2.625	30.514	1.00	35.87
88	CA	ASP	A	823	-28.538	3.85	30.921	1.00	35.01
89	C	ASP	A	823	-29.66	4.201	29.945	1.00	33.26
90	O	ASP	A	823	-30.427	5.126	30.187	1.00	34.38
91	CB	ASP	A	823	-27.562	5.031	30.982	1.00	37.74
92	CG	ASP	A	823	-26.597	4.948	32.154	1.00	39.24
93	OD1	ASP	A	823	-27.055	4.719	33.296	1.00	39.21
94	OD2	ASP	A	823	-25.381	5.13	31.93	1.00	39.6
95	N	ILE	A	824	-29.75	3.476	28.837	1.00	30.38
96	CA	ILE	A	824	-30.783	3.757	27.855	1.00	28.22
97	C	ILE	A	824	-32.023	2.907	28.092	1.00	28.73
98	O	ILE	A	824	-31.94	1.694	28.275	1.00	29.99
99	CB	ILE	A	824	-30.283	3.499	26.421	1.00	27.37
100	CG1	ILE	A	824	-29	4.289	26.165	1.00	25.79
101	CG2	ILE	A	824	-31.359	3.899	25.418	1.00	24.89
102	CD1	ILE	A	824	-28.31	3.925	24.864	1.00	25.05
103	N	LYS	A	825	-33.174	3.56	28.09	1.00	27.88
104	CA	LYS	A	825	-34.436	2.878	28.287	1.00	27.9
105	C	LYS	A	825	-35.342	3.262	27.123	1.00	27.3
106	O	LYS	A	825	-35.751	4.413	27.008	1.00	28.19
107	CB	LYS	A	825	-35.063	3.305	29.616	1.00	29.1
108	CG	LYS	A	825	-36.376	2.606	29.955	1.00	31.89
109	CD	LYS	A	825	-36.875	3.053	31.318	1.00	35.72
110	CE	LYS	A	825	-38.144	2.329	31.727	1.00	37.53
111	NZ	LYS	A	825	-38.624	2.79	33.065	1.00	38.55
112	N	PHE	A	826	-35.635	2.297	26.256	1.00	26.32
113	CA	PHE	A	826	-36.488	2.536	25.1	1.00	24.98
114	C	PHE	A	826	-37.956	2.53	25.512	1.00	25.38
115	O	PHE	A	826	-38.419	1.598	26.174	1.00	24.9
116	CB	PHE	A	826	-36.228	1.471	24.038	1.00	22.71
117	CG	PHE	A	826	-34.787	1.379	23.622	1.00	23.84
118	CD1	PHE	A	826	-33.971	0.357	24.104	1.00	23.4
119	CD2	PHE	A	826	-34.237	2.324	22.758	1.00	20.67

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

120	CE1	PHE	A	826	-32.63	0.283	23.728	1.00	21.64
121	CE2	PHE	A	826	-32.906	2.256	22.38	1.00	20.18
122	CZ	PHE	A	826	-32.101	1.236	22.864	1.00	22.03
123	N	GLN	A	827	-38.688	3.565	25.108	1.00	24.49
124	CA	GLN	A	827	-40.094	3.685	25.475	1.00	27.08
125	C	GLN	A	827	-41.069	3.515	24.318	1.00	27.52
126	O	GLN	A	827	-42.177	3.02	24.513	1.00	27.61
127	CB	GLN	A	827	-40.35	5.044	26.132	1.00	28.44
128	CG	GLN	A	827	-39.174	5.585	26.937	1.00	31.01
129	CD	GLN	A	827	-39.401	7.011	27.414	1.00	32.09
130	OE1	GLN	A	827	-39.965	7.238	28.486	1.00	34.37
131	NE2	GLN	A	827	-38.976	7.98	26.609	1.00	32.3
132	N	ASP	A	828	-40.673	3.92	23.116	1.00	28.52
133	CA	ASP	A	828	-41.576	3.805	21.975	1.00	29.38
134	C	ASP	A	828	-40.874	4.046	20.638	1.00	30.67
135	O	ASP	A	828	-39.701	4.421	20.591	1.00	31.56
136	CB	ASP	A	828	-42.724	4.81	22.145	1.00	29.71
137	CG	ASP	A	828	-43.893	4.542	21.208	1.00	30.52
138	OD1	ASP	A	828	-43.811	3.614	20.376	1.00	30.87
139	OD2	ASP	A	828	-44.901	5.269	21.311	1.00	29.95
140	N	VAL	A	829	-41.603	3.814	19.55	1.00	30.65
141	CA	VAL	A	829	-41.086	4.02	18.202	1.00	29.59
142	C	VAL	A	829	-41.83	5.206	17.592	1.00	28.66
143	O	VAL	A	829	-43.06	5.259	17.612	1.00	28.97
144	CB	VAL	A	829	-41.311	2.772	17.32	1.00	29.9
145	CG1	VAL	A	829	-40.817	3.032	15.91	1.00	29.09
146	CG2	VAL	A	829	-40.585	1.577	17.921	1.00	31.03
147	N	ILE	A	830	-41.085	6.163	17.055	1.00	27.59
148	CA	ILE	A	830	-41.699	7.341	16.459	1.00	26.69
149	C	ILE	A	830	-40.897	7.803	15.255	1.00	25.93
150	O	ILE	A	830	-39.824	7.272	14.971	1.00	26.18
151	CB	ILE	A	830	-41.753	8.525	17.46	1.00	27.51
152	CG1	ILE	A	830	-40.332	9.002	17.782	1.00	27.05
153	CG2	ILE	A	830	-42.472	8.107	18.745	1.00	27.09
154	CD1	ILE	A	830	-40.289	10.279	18.628	1.00	27.24
155	N	GLY	A	831	-41.426	8.799	14.552	1.00	24.54
156	CA	GLY	A	831	-40.727	9.339	13.402	1.00	22.44
157	C	GLY	A	831	-40.14	10.692	13.758	1.00	20.7
158	O	GLY	A	831	-40.643	11.377	14.652	1.00	20.57
159	N	GLU	A	832	-39.065	11.08	13.083	1.00	18.23

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

160	CA	GLU	A	832	-38.455	12.374	13.352	1.00	17.41
161	C	GLU	A	832	-37.828	12.953	12.095	1.00	15.62
162	O	GLU	A	832	-36.613	12.915	11.919	1.00	15.21
163	CB	GLU	A	832	-37.401	12.273	14.468	1.00	16.38
164	CG	GLU	A	832	-36.931	13.639	14.963	1.00	17.64
165	CD	GLU	A	832	-36.298	13.591	16.341	1.00	19.51
166	OE1	GLU	A	832	-36.746	12.771	17.171	1.00	21.35
167	OE2	GLU	A	832	-35.369	14.382	16.605	1.00	19.85
168	N	GLY	A	833	-38.674	13.494	11.226	1.00	15.66
169	CA	GLY	A	833	-38.197	14.081	9.987	1.00	15.3
170	C	GLY	A	833	-37.37	13.125	9.146	1.00	15.92
171	O	GLY	A	833	-37.683	11.932	9.054	1.00	14.36
172	N	ASN	A	834	-36.302	13.648	8.544	1.00	15.15
173	CA	ASN	A	834	-35.443	12.845	7.692	1.00	14.91
174	C	ASN	A	834	-34.629	11.802	8.455	1.00	16.09
175	O	ASN	A	834	-33.816	11.089	7.863	1.00	16.75
176	CB	ASN	A	834	-34.525	13.75	6.85	1.00	14.16
177	CG	ASN	A	834	-33.67	14.687	7.693	1.00	14.14
178	OD1	ASN	A	834	-32.992	15.569	7.157	1.00	14.07
179	ND2	ASN	A	834	-33.696	14.503	9.012	1.00	11.54
180	N	PHE	A	835	-34.836	11.717	9.768	1.00	15.58
181	CA	PHE	A	835	-34.142	10.711	10.568	1.00	15.36
182	C	PHE	A	835	-34.889	9.398	10.361	1.00	17.57
183	O	PHE	A	835	-34.359	8.316	10.62	1.00	17.3
184	CB	PHE	A	835	-34.176	11.047	12.065	1.00	13.96
185	CG	PHE	A	835	-33.12	12.022	12.504	1.00	14.93
186	CD1	PHE	A	835	-33.371	13.394	12.507	1.00	15.03
187	CD2	PHE	A	835	-31.874	11.567	12.925	1.00	13.37
188	CE1	PHE	A	835	-32.392	14.298	12.926	1.00	15.27
189	CE2	PHE	A	835	-30.891	12.457	13.344	1.00	13.87
190	CZ	PHE	A	835	-31.147	13.824	13.346	1.00	15.94
191	N	GLY	A	836	-36.129	9.506	9.891	1.00	18.27
192	CA	GLY	A	836	-36.944	8.329	9.68	1.00	19.06
193	C	GLY	A	836	-37.507	7.898	11.017	1.00	21.87
194	O	GLY	A	836	-37.787	8.739	11.877	1.00	22.14
195	N	GLN	A	837	-37.669	6.594	11.204	1.00	23.14
196	CA	GLN	A	837	-38.198	6.068	12.455	1.00	24.49
197	C	GLN	A	837	-37.089	6.006	13.498	1.00	22.41
198	O	GLN	A	837	-35.997	5.512	13.223	1.00	23.03
199	CB	GLN	A	837	-38.78	4.669	12.236	1.00	27.79



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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

200	CG	GLN	A	837	-39.871	4.619	11.175	1.00	35.51
201	CD	GLN	A	837	-41.069	5.503	11.511	1.00	39.76
202	OE1	GLN	A	837	-41.786	5.259	12.486	1.00	42.8
203	NE2	GLN	A	837	-41.287	6.535	10.701	1.00	39.23
204	N	VAL	A	838	-37.371	6.518	14.689	1.00	18.47
205	CA	VAL	A	838	-36.399	6.515	15.77	1.00	17.84
206	C	VAL	A	838	-37.082	5.961	17.005	1.00	18.75
207	O	VAL	A	838	-38.301	5.804	17.029	1.00	19.03
208	CB	VAL	A	838	-35.87	7.947	16.086	1.00	16.81
209	CG1	VAL	A	838	-35.187	8.527	14.875	1.00	16.6
210	CG2	VAL	A	838	-37.005	8.849	16.525	1.00	15.46
211	N	LEU	A	839	-36.3	5.66	18.03	1.00	19.77
212	CA	LEU	A	839	-36.86	5.128	19.264	1.00	21.43
213	C	LEU	A	839	-36.967	6.222	20.322	1.00	21.62
214	O	LEU	A	839	-35.984	6.895	20.628	1.00	20.32
215	CB	LEU	A	839	-35.975	3.997	19.79	1.00	21.74
216	CG	LEU	A	839	-35.839	2.756	18.906	1.00	22.24
217	CD1	LEU	A	839	-34.608	1.971	19.307	1.00	22.29
218	CD2	LEU	A	839	-37.089	1.903	19.036	1.00	22.01
219	N	LYS	A	840	-38.164	6.423	20.86	1.00	23.49
220	CA	LYS	A	840	-38.325	7.416	21.908	1.00	26.57
221	C	LYS	A	840	-37.734	6.745	23.136	1.00	26.7
222	O	LYS	A	840	-38.055	5.596	23.44	1.00	27.01
223	CB	LYS	A	840	-39.799	7.743	22.165	1.00	28.16
224	CG	LYS	A	840	-40	8.806	23.259	1.00	30.27
225	CD	LYS	A	840	-41.463	9.207	23.395	1.00	32.7
226	CE	LYS	A	840	-41.676	10.25	24.495	1.00	34.42
227	NZ	LYS	A	840	-41.438	9.728	25.881	1.00	34.83
228	N	ALA	A	841	-36.861	7.449	23.837	1.00	26.22
229	CA	ALA	A	841	-36.248	6.857	25.007	1.00	26.99
230	C	ALA	A	841	-35.776	7.89	26.008	1.00	26.75
231	O	ALA	A	841	-35.885	9.096	25.787	1.00	26.39
232	CB	ALA	A	841	-35.075	5.986	24.576	1.00	26.08
233	N	ARG	A	842	-35.269	7.391	27.126	1.00	28.34
234	CA	ARG	A	842	-34.721	8.237	28.168	1.00	28.68
235	C	ARG	A	842	-33.278	7.797	28.332	1.00	28.63
236	O	ARG	A	842	-32.983	6.604	28.391	1.00	28.09
237	CB	ARG	A	842	-35.478	8.058	29.483	1.00	29.11
238	CG	ARG	A	842	-36.92	8.51	29.426	1.00	30.27
239	CD	ARG	A	842	-37.368	8.992	30.783	1.00	34.48

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

240	NE	ARG	A	842	-36.601	10.156	31.219	1.00	38.28
241	CZ	ARG	A	842	-36.752	10.754	32.398	1.00	41.3
242	NH1	ARG	A	842	-37.645	10.298	33.267	1.00	42.24
243	NH2	ARG	A	842	-36.013	11.813	32.71	1.00	43.29
244	N	ILE	A	843	-32.373	8.764	28.36	1.00	29.63
245	CA	ILE	A	843	-30.961	8.463	28.528	1.00	29.63
246	C	ILE	A	843	-30.467	9.187	29.768	1.00	30.76
247	O	ILE	A	843	-31.217	9.928	30.412	1.00	30.17
248	CB	ILE	A	843	-30.128	8.939	27.313	1.00	27.85
249	CG1	ILE	A	843	-30.249	10.46	27.158	1.00	27.52
250	CG2	ILE	A	843	-30.603	8.234	26.05	1.00	27.47
251	CD1	ILE	A	843	-29.277	11.058	26.156	1.00	26.6
252	N	LYS	A	844	-29.205	8.959	30.103	1.00	33.32
253	CA	LYS	A	844	-28.599	9.612	31.246	1.00	36.06
254	C	LYS	A	844	-27.48	10.497	30.712	1.00	37.65
255	O	LYS	A	844	-26.464	10	30.222	1.00	38.47
256	CB	LYS	A	844	-28.032	8.582	32.227	1.00	37.08
257	CG	LYS	A	844	-27.417	9.204	33.483	1.00	40.55
258	CD	LYS	A	844	-27.02	8.148	34.521	1.00	42.35
259	CE	LYS	A	844	-26.457	8.794	35.789	1.00	42.89
260	NZ	LYS	A	844	-26.105	7.799	36.851	1.00	41.44
261	N	LYS	A	845	-27.688	11.809	30.771	1.00	37.52
262	CA	LYS	A	845	-26.679	12.744	30.311	1.00	38.95
263	C	LYS	A	845	-26.394	13.748	31.421	1.00	38.61
264	O	LYS	A	845	-27.313	14.312	32.017	1.00	37.33
265	CB	LYS	A	845	-27.136	13.473	29.043	1.00	39.57
266	CG	LYS	A	845	-26.031	14.33	28.438	1.00	41.46
267	CD	LYS	A	845	-26.446	15.022	27.154	1.00	42.42
268	CE	LYS	A	845	-25.265	15.774	26.558	1.00	42.06
269	NZ	LYS	A	845	-25.646	16.562	25.356	1.00	44.39
270	N	ASP	A	846	-25.111	13.963	31.692	1.00	38.58
271	CA	ASP	A	846	-24.694	14.884	32.736	1.00	38.73
272	C	ASP	A	846	-25.312	14.478	34.072	1.00	37.9
273	O	ASP	A	846	-25.758	15.321	34.849	1.00	37.26
274	CB	ASP	A	846	-25.1	16.317	32.369	1.00	40.58
275	CG	ASP	A	846	-24.393	16.823	31.115	1.00	41.95
276	OD1	ASP	A	846	-23.144	16.74	31.062	1.00	41.05
277	OD2	ASP	A	846	-25.084	17.308	30.189	1.00	41.47
278	N	GLY	A	847	-25.346	13.172	34.322	1.00	37.12
279	CA	GLY	A	847	-25.896	12.664	35.566	1.00	35.87

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

280	C	GLY	A	847	-27.404	12.764	35.7	1.00	35.64
281	O	GLY	A	847	-27.973	12.284	36.679	1.00	36.61
282	N	LEU	A	848	-28.064	13.379	34.728	1.00	34.72
283	CA	LEU	A	848	-29.511	13.514	34.794	1.00	34.13
284	C	LEU	A	848	-30.238	12.643	33.786	1.00	34.45
285	O	LEU	A	848	-29.738	12.369	32.695	1.00	34.93
286	CB	LEU	A	848	-29.925	14.969	34.577	1.00	33.54
287	CG	LEU	A	848	-29.569	15.968	35.678	1.00	35.26
288	CD1	LEU	A	848	-30.154	17.331	35.329	1.00	34.2
289	CD2	LEU	A	848	-30.121	15.481	37.021	1.00	34.82
290	N	ARG	A	849	-31.428	12.204	34.166	1.00	33.9
291	CA	ARG	A	849	-32.249	11.394	33.289	1.00	33.85
292	C	ARG	A	849	-33.031	12.381	32.425	1.00	32.3
293	O	ARG	A	849	-33.546	13.378	32.932	1.00	31.6
294	CB	ARG	A	849	-33.191	10.527	34.122	1.00	34.96
295	CG	ARG	A	849	-32.461	9.484	34.973	1.00	37.55
296	CD	ARG	A	849	-32.003	8.316	34.126	1.00	39.5
297	NE	ARG	A	849	-33.146	7.597	33.564	1.00	42.56
298	CZ	ARG	A	849	-33.065	6.703	32.582	1.00	43.86
299	NH1	ARG	A	849	-34.165	6.099	32.141	1.00	44.1
300	NH2	ARG	A	849	-31.888	6.417	32.036	1.00	42.25
301	N	MET	A	850	-33.101	12.121	31.123	1.00	29.69
302	CA	MET	A	850	-33.812	13.024	30.229	1.00	26.84
303	C	MET	A	850	-34.414	12.312	29.033	1.00	25.34
304	O	MET	A	850	-34.046	11.187	28.716	1.00	26.76
305	CB	MET	A	850	-32.865	14.111	29.723	1.00	25.67
306	CG	MET	A	850	-31.792	13.587	28.788	1.00	26.81
307	SD	MET	A	850	-30.685	14.862	28.186	1.00	28.08
308	CE	MET	A	850	-31.649	15.535	26.842	1.00	28.71
309	N	ASP	A	851	-35.34	12.99	28.368	1.00	24.94
310	CA	ASP	A	851	-35.991	12.453	27.182	1.00	23.8
311	C	ASP	A	851	-35.076	12.609	25.973	1.00	22.65
312	O	ASP	A	851	-34.238	13.515	25.921	1.00	21.26
313	CB	ASP	A	851	-37.301	13.198	26.913	1.00	25.23
314	CG	ASP	A	851	-38.386	12.854	27.913	1.00	26.56
315	OD1	ASP	A	851	-39.451	13.497	27.864	1.00	28.06
316	OD2	ASP	A	851	-38.181	11.937	28.74	1.00	28.96
317	N	ALA	A	852	-35.237	11.718	25.003	1.00	21.33
318	CA	ALA	A	852	-34.441	11.768	23.784	1.00	20.69
319	C	ALA	A	852	-34.978	10.766	22.776	1.00	19.78

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

320	O	ALA	A	852	-35.902	10.001	23.067	1.00	19.69
321	CB	ALA	A	852	-32.975	11.467	24.094	1.00	19.65
322	N	ALA	A	853	-34.407	10.786	21.581	1.00	18.74
323	CA	ALA	A	853	-34.81	9.862	20.537	1.00	18.78
324	C	ALA	A	853	-33.537	9.151	20.115	1.00	19.69
325	O	ALA	A	853	-32.448	9.725	20.182	1.00	19.58
326	CB	ALA	A	853	-35.414	10.614	19.37	1.00	18.86
327	N	ILE	A	854	-33.659	7.9	19.694	1.00	19.87
328	CA	ILE	A	854	-32.478	7.159	19.292	1.00	19.24
329	C	ILE	A	854	-32.593	6.571	17.894	1.00	20.24
330	O	ILE	A	854	-33.555	5.879	17.561	1.00	19.26
331	CB	ILE	A	854	-32.153	6.065	20.334	1.00	18.3
332	CG1	ILE	A	854	-31.766	6.746	21.65	1.00	16.44
333	CG2	ILE	A	854	-31.034	5.162	19.835	1.00	15.03
334	CD1	ILE	A	854	-31.21	5.833	22.693	1.00	18.32
335	N	LYS	A	855	-31.595	6.889	17.078	1.00	22.15
336	CA	LYS	A	855	-31.51	6.44	15.699	1.00	22.14
337	C	LYS	A	855	-30.472	5.337	15.591	1.00	23.11
338	O	LYS	A	855	-29.281	5.59	15.753	1.00	22.18
339	CB	LYS	A	855	-31.09	7.61	14.805	1.00	21.82
340	CG	LYS	A	855	-30.792	7.234	13.353	1.00	20.39
341	CD	LYS	A	855	-32.032	6.759	12.621	1.00	16.85
342	CE	LYS	A	855	-31.721	6.545	11.151	1.00	17.67
343	NZ	LYS	A	855	-32.91	6.163	10.338	1.00	15.41
344	N	ARG	A	856	-30.923	4.116	15.319	1.00	25.15
345	CA	ARG	A	856	-30.008	2.996	15.174	1.00	27.37
346	C	ARG	A	856	-29.419	3.001	13.763	1.00	28.22
347	O	ARG	A	856	-30.147	3.016	12.771	1.00	27.32
348	CB	ARG	A	856	-30.728	1.669	15.431	1.00	29.11
349	CG	ARG	A	856	-29.759	0.516	15.644	1.00	33.11
350	CD	ARG	A	856	-30.457	-0.791	15.953	1.00	34.74
351	NE	ARG	A	856	-31.169	-1.308	14.792	1.00	38.39
352	CZ	ARG	A	856	-31.169	-2.585	14.429	1.00	39.5
353	NH1	ARG	A	856	-30.488	-3.479	15.138	1.00	39.22
354	NH2	ARG	A	856	-31.85	-2.966	13.354	1.00	41.26
355	N	MET	A	857	-28.095	2.997	13.684	1.00	30.08
356	CA	MET	A	857	-27.398	3.011	12.409	1.00	32.76
357	C	MET	A	857	-26.557	1.758	12.243	1.00	36.75
358	O	MET	A	857	-25.798	1.381	13.142	1.00	36.43
359	CB	MET	A	857	-26.505	4.251	12.321	1.00	31.36

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

360	CG	MET	A	857	-27.288	5.556	12.211	1.00	31.22
361	SD	MET	A	857	-26.302	7.049	12.451	1.00	30.64
362	CE	MET	A	857	-25.222	6.987	10.979	1.00	29.88
363	N	ALA	A	858	-26.702	1.112	11.09	1.00	41.07
364	CA	ALA	A	858	-25.952	-0.101	10.789	1.00	45.33
365	C	ALA	A	858	-24.539	0.264	10.338	1.00	48.15
366	O	ALA	A	858	-24.342	0.761	9.229	1.00	47.58
367	CB	ALA	A	858	-26.663	-0.9	9.701	1.00	45.69
368	N	GLU	A	859	-23.562	0.018	11.209	1.00	51.59
369	CA	GLU	A	859	-22.167	0.325	10.911	1.00	55.03
370	C	GLU	A	859	-21.646	-0.482	9.727	1.00	57.12
371	O	GLU	A	859	-21.003	0.066	8.827	1.00	57.62
372	CB	GLU	A	859	-21.295	0.058	12.141	1.00	55.64
373	CG	GLU	A	859	-21.643	0.926	13.335	1.00	56.6
374	CD	GLU	A	859	-20.746	0.662	14.524	1.00	57.29
375	OE1	GLU	A	859	-20.679	-0.502	14.966	1.00	58.08
376	OE2	GLU	A	859	-20.111	1.618	15.019	1.00	57.75
377	N	ALA	A	860	-21.919	-1.782	9.732	1.00	58.88
378	CA	ALA	A	860	-21.475	-2.651	8.648	1.00	60.93
379	CB	ALA	A	860	-21.128	-4.038	9.196	1.00	60.99
380	C	ALA	A	860	-22.57	-2.756	7.584	1.00	62.06
381	OT1	ALA	A	860	-22.925	-3.897	7.206	1.00	62.65
382	OT2	ALA	A	860	-23.056	-1.69	7.138	1.00	61.95
383	N	ALA	A	867	-17.273	3.609	3.614	1.00	61.13
384	CA	ALA	A	867	-18.606	3.014	3.922	1.00	60.5
385	C	ALA	A	867	-19.709	4.061	3.812	1.00	60.05
386	O	ALA	A	867	-19.474	5.255	4.016	1.00	59.71
387	CB	ALA	A	867	-18.599	2.409	5.328	1.00	59.9
388	N	ASP	A	868	-20.911	3.601	3.478	1.00	59.69
389	CA	ASP	A	868	-22.075	4.471	3.351	1.00	59.47
390	C	ASP	A	868	-22.405	5.005	4.749	1.00	58.62
391	O	ASP	A	868	-23.091	6.016	4.905	1.00	58.55
392	CB	ASP	A	868	-23.256	3.665	2.806	1.00	60.42
393	CG	ASP	A	868	-24.407	4.537	2.362	1.00	61.77
394	OD1	ASP	A	868	-24.846	5.397	3.157	1.00	63.14
395	OD2	ASP	A	868	-24.877	4.354	1.218	1.00	62.11
396	N	PHE	A	869	-21.893	4.301	5.756	1.00	56.76
397	CA	PHE	A	869	-22.081	4.64	7.162	1.00	54.42
398	C	PHE	A	869	-21.134	5.763	7.59	1.00	53.23
399	O	PHE	A	869	-21.562	6.773	8.148	1.00	52.84

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

400	CB	PHE	A	869	-21.821	3.395	8.016	1.00	53.87
401	CG	PHE	A	869	-21.729	3.672	9.487	1.00	52.76
402	CD1	PHE	A	869	-22.877	3.842	10.251	1.00	52.87
403	CD2	PHE	A	869	-20.488	3.771	10.108	1.00	52.17
404	CE1	PHE	A	869	-22.791	4.105	11.617	1.00	52.66
405	CE2	PHE	A	869	-20.388	4.035	11.469	1.00	52.35
406	CZ	PHE	A	869	-21.542	4.202	12.227	1.00	52.69
407	N	ALA	A	870	-19.843	5.571	7.332	1.00	51.77
408	CA	ALA	A	870	-18.829	6.559	7.689	1.00	49.7
409	C	ALA	A	870	-19.092	7.884	6.984	1.00	48.21
410	O	ALA	A	870	-18.622	8.937	7.424	1.00	47.33
411	CB	ALA	A	870	-17.446	6.04	7.324	1.00	48.69
412	N	GLY	A	871	-19.841	7.821	5.888	1.00	46.52
413	CA	GLY	A	871	-20.161	9.021	5.138	1.00	45.11
414	C	GLY	A	871	-21.074	9.953	5.912	1.00	44.19
415	O	GLY	A	871	-20.72	11.098	6.178	1.00	42.85
416	N	GLU	A	872	-22.252	9.459	6.278	1.00	44.2
417	CA	GLU	A	872	-23.217	10.253	7.025	1.00	44.63
418	C	GLU	A	872	-22.762	10.549	8.447	1.00	43.24
419	O	GLU	A	872	-23.14	11.569	9.026	1.00	43.24
420	CB	GLU	A	872	-24.575	9.552	7.05	1.00	46.63
421	CG	GLU	A	872	-24.526	8.084	6.702	1.00	49.68
422	CD	GLU	A	872	-25.91	7.488	6.571	1.00	53.07
423	OE1	GLU	A	872	-26.607	7.379	7.602	1.00	54.55
424	OE2	GLU	A	872	-26.306	7.138	5.438	1.00	55.27
425	N	LEU	A	873	-21.955	9.657	9.008	1.00	41.96
426	CA	LEU	A	873	-21.441	9.842	10.357	1.00	42.08
427	C	LEU	A	873	-20.45	11.006	10.331	1.00	41.81
428	O	LEU	A	873	-20.374	11.804	11.264	1.00	41.14
429	CB	LEU	A	873	-20.747	8.563	10.83	1.00	43.07
430	CG	LEU	A	873	-20.223	8.544	12.266	1.00	43.78
431	CD1	LEU	A	873	-21.367	8.786	13.243	1.00	43.16
432	CD2	LEU	A	873	-19.569	7.2	12.541	1.00	44.84
433	N	GLU	A	874	-19.699	11.093	9.239	1.00	42.55
434	CA	GLU	A	874	-18.713	12.147	9.037	1.00	42.99
435	C	GLU	A	874	-19.415	13.505	8.961	1.00	40.89
436	O	GLU	A	874	-18.881	14.517	9.414	1.00	41.21
437	CB	GLU	A	874	-17.948	11.884	7.736	1.00	46.01
438	CG	GLU	A	874	-16.86	12.896	7.398	1.00	49.68
439	CD	GLU	A	874	-16.358	12.744	5.965	1.00	52.28

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

440	OE1	GLU	A	874	-15.996	11.613	5.57	1.00	53.65
441	OE2	GLU	A	874	-16.325	13.757	5.232	1.00	53.05
442	N	VAL	A	875	-20.612	13.519	8.382	1.00	38.35
443	CA	VAL	A	875	-21.382	14.751	8.252	1.00	35.04
444	C	VAL	A	875	-22.05	15.134	9.567	1.00	33.74
445	O	VAL	A	875	-22.088	16.308	9.923	1.00	33.14
446	CB	VAL	A	875	-22.467	14.628	7.16	1.00	34.06
447	CG1	VAL	A	875	-23.282	15.912	7.089	1.00	31.12
448	CG2	VAL	A	875	-21.815	14.339	5.811	1.00	30.28
449	N	LEU	A	876	-22.572	14.146	10.288	1.00	31.89
450	CA	LEU	A	876	-23.228	14.404	11.567	1.00	31.95
451	C	LEU	A	876	-22.297	15.038	12.603	1.00	32.57
452	O	LEU	A	876	-22.751	15.758	13.493	1.00	32.47
453	CB	LEU	A	876	-23.808	13.106	12.135	1.00	30.87
454	CG	LEU	A	876	-25.024	12.538	11.401	1.00	30.58
455	CD1	LEU	A	876	-25.344	11.142	11.923	1.00	30.45
456	CD2	LEU	A	876	-26.21	13.478	11.586	1.00	29.06
457	N	CYS	A	877	-20.999	14.77	12.49	1.00	32.84
458	CA	CYS	A	877	-20.021	15.316	13.427	1.00	34.69
459	C	CYS	A	877	-19.703	16.775	13.156	1.00	33.62
460	O	CYS	A	877	-19.253	17.496	14.046	1.00	34.42
461	CB	CYS	A	877	-18.72	14.511	13.381	1.00	36.71
462	SG	CYS	A	877	-18.824	12.914	14.2	1.00	43.15
463	N	LYS	A	878	-19.934	17.204	11.925	1.00	30.97
464	CA	LYS	A	878	-19.667	18.577	11.544	1.00	29.83
465	C	LYS	A	878	-20.856	19.483	11.854	1.00	27.75
466	O	LYS	A	878	-20.823	20.678	11.564	1.00	28.14
467	CB	LYS	A	878	-19.337	18.643	10.051	1.00	31.56
468	CG	LYS	A	878	-18.19	17.741	9.637	1.00	32.79
469	CD	LYS	A	878	-16.875	18.178	10.263	1.00	35.97
470	CE	LYS	A	878	-15.796	17.116	10.048	1.00	39.95
471	NZ	LYS	A	878	-15.692	16.707	8.609	1.00	40.08
472	N	LEU	A	879	-21.903	18.916	12.445	1.00	25.9
473	CA	LEU	A	879	-23.097	19.69	12.775	1.00	25.24
474	C	LEU	A	879	-22.877	20.706	13.883	1.00	24.73
475	O	LEU	A	879	-23.311	21.846	13.776	1.00	26.78
476	CB	LEU	A	879	-24.248	18.765	13.19	1.00	23.04
477	CG	LEU	A	879	-25.018	18.021	12.098	1.00	22.7
478	CD1	LEU	A	879	-25.995	17.043	12.737	1.00	21.25
479	CD2	LEU	A	879	-25.754	19.023	11.21	1.00	21.51

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## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

480	N	GLY	A	880	-22.204	20.295	14.949	1.00	24.67
481	CA	GLY	A	880	-21.998	21.201	16.06	1.00	24.4
482	C	GLY	A	880	-23.323	21.372	16.786	1.00	24.23
483	O	GLY	A	880	-24.169	20.476	16.765	1.00	23.05
484	N	HIS	A	881	-23.521	22.522	17.419	1.00	23.09
485	CA	HIS	A	881	-24.759	22.764	18.137	1.00	22.66
486	C	HIS	A	881	-25.366	24.111	17.805	1.00	20.85
487	O	HIS	A	881	-24.662	25.086	17.536	1.00	19.82
488	CB	HIS	A	881	-24.532	22.673	19.648	1.00	25.37
489	CG	HIS	A	881	-24.22	21.291	20.125	1.00	31.01
490	ND1	HIS	A	881	-25.174	20.299	20.204	1.00	34.35
491	CD2	HIS	A	881	-23.054	20.724	20.518	1.00	32.77
492	CE1	HIS	A	881	-24.61	19.18	20.626	1.00	34.12
493	NE2	HIS	A	881	-23.324	19.412	20.823	1.00	35.69
494	N	HIS	A	882	-26.692	24.137	17.814	1.00	17.26
495	CA	HIS	A	882	-27.456	25.336	17.555	1.00	15.3
496	C	HIS	A	882	-28.878	25.004	17.97	1.00	15.66
497	O	HIS	A	882	-29.355	23.886	17.754	1.00	14.51
498	CB	HIS	A	882	-27.399	25.723	16.079	1.00	15.3
499	CG	HIS	A	882	-28.04	27.043	15.784	1.00	16.18
500	ND1	HIS	A	882	-29.407	27.226	15.79	1.00	16.47
501	CD2	HIS	A	882	-27.499	28.258	15.524	1.00	14.54
502	CE1	HIS	A	882	-29.68	28.496	15.549	1.00	16.12
503	NE2	HIS	A	882	-28.54	29.144	15.385	1.00	16.13
504	N	PRO	A	883	-29.568	25.966	18.597	1.00	14.55
505	CA	PRO	A	883	-30.947	25.808	19.069	1.00	13.45
506	C	PRO	A	883	-31.952	25.41	17.991	1.00	12.43
507	O	PRO	A	883	-32.922	24.692	18.269	1.00	10.95
508	CB	PRO	A	883	-31.269	27.184	19.657	1.00	14.12
509	CG	PRO	A	883	-29.938	27.679	20.112	1.00	15.53
510	CD	PRO	A	883	-29.048	27.296	18.948	1.00	13.81
511	N	ASN	A	884	-31.718	25.868	16.764	1.00	10.12
512	CA	ASN	A	884	-32.647	25.59	15.677	1.00	9.94
513	C	ASN	A	884	-32.37	24.386	14.775	1.00	10.41
514	O	ASN	A	884	-32.87	24.324	13.651	1.00	10.94
515	CB	ASN	A	884	-32.829	26.862	14.845	1.00	9.71
516	CG	ASN	A	884	-33.343	28.029	15.687	1.00	10.4
517	OD1	ASN	A	884	-32.783	29.126	15.665	1.00	7.91
518	ND2	ASN	A	884	-34.413	27.788	16.435	1.00	8.55
519	N	ILE	A	885	-31.556	23.448	15.251	1.00	10.49



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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

520	CA	ILE	A	885	-31.305	22.209	14.508	1.00	11.94
521	C	ILE	A	885	-31.481	21.118	15.548	1.00	11.87
522	O	ILE	A	885	-31.519	21.41	16.74	1.00	12.4
523	CB	ILE	A	885	-29.867	22.078	13.926	1.00	12.26
524	CG1	ILE	A	885	-28.85	21.93	15.06	1.00	13.72
525	CG2	ILE	A	885	-29.547	23.266	13.006	1.00	10.68
526	CD1	ILE	A	885	-27.423	21.661	14.559	1.00	12.71
527	N	ILE	A	886	-31.64	19.878	15.108	1.00	11.27
528	CA	ILE	A	886	-31.771	18.78	16.049	1.00	10.72
529	C	ILE	A	886	-30.345	18.499	16.479	1.00	10.83
530	O	ILE	A	886	-29.499	18.178	15.657	1.00	9.8
531	CB	ILE	A	886	-32.374	17.513	15.38	1.00	12.36
532	CG1	ILE	A	886	-33.868	17.724	15.112	1.00	10.83
533	CG2	ILE	A	886	-32.157	16.288	16.264	1.00	8.87
534	CD1	ILE	A	886	-34.72	17.82	16.362	1.00	7.06
535	N	ASN	A	887	-30.079	18.634	17.768	1.00	11.62
536	CA	ASN	A	887	-28.744	18.406	18.287	1.00	13.94
537	C	ASN	A	887	-28.465	16.959	18.684	1.00	15.68
538	O	ASN	A	887	-29.362	16.235	19.125	1.00	14.49
539	CB	ASN	A	887	-28.506	19.338	19.476	1.00	14.46
540	CG	ASN	A	887	-28.437	20.795	19.057	1.00	15.16
541	OD1	ASN	A	887	-27.417	21.253	18.541	1.00	15.85
542	ND2	ASN	A	887	-29.535	21.526	19.249	1.00	15.67
543	N	LEU	A	888	-27.22	16.532	18.493	1.00	17.86
544	CA	LEU	A	888	-26.821	15.184	18.87	1.00	19.79
545	C	LEU	A	888	-26.529	15.224	20.37	1.00	21.33
546	O	LEU	A	888	-25.898	16.16	20.857	1.00	21.16
547	CB	LEU	A	888	-25.575	14.746	18.098	1.00	20.12
548	CG	LEU	A	888	-25.637	14.695	16.565	1.00	21.77
549	CD1	LEU	A	888	-24.475	13.848	16.071	1.00	22.28
550	CD2	LEU	A	888	-26.95	14.096	16.085	1.00	20.81
551	N	LEU	A	889	-26.988	14.213	21.099	1.00	22.32
552	CA	LEU	A	889	-26.795	14.171	22.542	1.00	24.43
553	C	LEU	A	889	-25.737	13.168	22.988	1.00	26.58
554	O	LEU	A	889	-25.266	13.213	24.129	1.00	27.88
555	CB	LEU	A	889	-28.123	13.849	23.229	1.00	23.47
556	CG	LEU	A	889	-29.259	14.851	23.014	1.00	22.98
557	CD1	LEU	A	889	-30.537	14.346	23.685	1.00	19.64
558	CD2	LEU	A	889	-28.841	16.211	23.582	1.00	21.61
559	N	GLY	A	890	-25.37	12.266	22.087	1.00	28.58

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

560	CA	GLY	A	890	-24.376	11.257	22.403	1.00	31.01
561	C	GLY	A	890	-24.517	10.034	21.516	1.00	32.67
562	O	GLY	A	890	-25.335	10.012	20.592	1.00	31.69
563	N	ALA	A	891	-23.72	9.01	21.796	1.00	34.93
564	CA	ALA	A	891	-23.76	7.788	21.007	1.00	36.51
565	C	ALA	A	891	-23.326	6.588	21.833	1.00	38.42
566	O	ALA	A	891	-22.641	6.733	22.849	1.00	38.1
567	CB	ALA	A	891	-22.867	7.929	19.786	1.00	36.03
568	N	CYS	A	892	-23.734	5.405	21.382	1.00	40.35
569	CA	CYS	A	892	-23.409	4.157	22.058	1.00	41.75
570	C	CYS	A	892	-23.386	2.981	21.081	1.00	42.42
571	O	CYS	A	892	-24.404	2.66	20.464	1.00	42.42
572	CB	CYS	A	892	-24.431	3.883	23.163	1.00	41.34
573	SG	CYS	A	892	-24.26	2.246	23.919	1.00	43.25
574	N	GLU	A	893	-22.22	2.35	20.936	1.00	43.36
575	CA	GLU	A	893	-22.076	1.198	20.046	1.00	44.17
576	C	GLU	A	893	-22.569	-0.047	20.764	1.00	43.42
577	O	GLU	A	893	-22.219	-0.286	21.92	1.00	44
578	CB	GLU	A	893	-20.617	1.001	19.636	1.00	45.43
579	CG	GLU	A	893	-20.076	2.094	18.741	1.00	49.9
580	CD	GLU	A	893	-18.694	1.772	18.21	1.00	52.73
581	OE1	GLU	A	893	-17.792	1.496	19.032	1.00	53.71
582	OE2	GLU	A	893	-18.51	1.794	16.973	1.00	53.47
583	N	HIS	A	894	-23.38	-0.839	20.077	1.00	42.44
584	CA	HIS	A	894	-23.934	-2.045	20.671	1.00	42.11
585	C	HIS	A	894	-24.168	-3.101	19.594	1.00	43.05
586	O	HIS	A	894	-25.015	-2.932	18.714	1.00	41.89
587	CB	HIS	A	894	-25.25	-1.704	21.37	1.00	41.16
588	CG	HIS	A	894	-25.753	-2.777	22.283	1.00	40.37
589	ND1	HIS	A	894	-25.158	-3.064	23.492	1.00	41.58
590	CD2	HIS	A	894	-26.812	-3.615	22.176	1.00	40.74
591	CE1	HIS	A	894	-25.83	-4.03	24.092	1.00	41.88
592	NE2	HIS	A	894	-26.838	-4.382	23.314	1.00	41.17
593	N	ARG	A	895	-23.396	-4.183	19.669	1.00	44.28
594	CA	ARG	A	895	-23.49	-5.295	18.728	1.00	44.3
595	C	ARG	A	895	-23.444	-4.887	17.259	1.00	43.39
596	O	ARG	A	895	-24.336	-5.233	16.485	1.00	43.65
597	CB	ARG	A	895	-24.768	-6.094	18.983	1.00	46.37
598	CG	ARG	A	895	-24.961	-6.552	20.421	1.00	49.59
599	CD	ARG	A	895	-26.164	-7.471	20.502	1.00	53.03

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

600	NE	ARG	A	895	-27.214	-7.011	19.598	1.00	56.53
601	CZ	ARG	A	895	-28.35	-7.659	19.366	1.00	58.57
602	NH1	ARG	A	895	-29.236	-7.15	18.517	1.00	59.43
603	NH2	ARG	A	895	-28.605	-8.808	19.98	1.00	59.41
604	N	GLY	A	896	-22.403	-4.153	16.879	1.00	42.88
605	CA	GLY	A	896	-22.255	-3.739	15.495	1.00	42.48
606	C	GLY	A	896	-23.131	-2.581	15.059	1.00	42.68
607	O	GLY	A	896	-22.987	-2.061	13.945	1.00	43.2
608	N	TYR	A	897	-24.05	-2.178	15.927	1.00	41.16
609	CA	TYR	A	897	-24.937	-1.068	15.616	1.00	39.3
610	C	TYR	A	897	-24.593	0.136	16.495	1.00	37.34
611	O	TYR	A	897	-24.205	-0.023	17.653	1.00	36.08
612	CB	TYR	A	897	-26.395	-1.489	15.832	1.00	39.82
613	CG	TYR	A	897	-26.924	-2.501	14.826	1.00	40.31
614	CD1	TYR	A	897	-27.393	-2.095	13.576	1.00	39.89
615	CD2	TYR	A	897	-26.986	-3.862	15.14	1.00	41.01
616	CE1	TYR	A	897	-27.918	-3.018	12.664	1.00	40.89
617	CE2	TYR	A	897	-27.509	-4.794	14.234	1.00	40.66
618	CZ	TYR	A	897	-27.976	-4.367	13	1.00	41.67
619	OH	TYR	A	897	-28.515	-5.281	12.111	1.00	41.66
620	N	LEU	A	898	-24.711	1.337	15.931	1.00	36.04
621	CA	LEU	A	898	-24.433	2.564	16.67	1.00	32.58
622	C	LEU	A	898	-25.749	3.217	17.05	1.00	31.53
623	O	LEU	A	898	-26.553	3.54	16.185	1.00	33.3
624	CB	LEU	A	898	-23.628	3.543	15.822	1.00	31.97
625	CG	LEU	A	898	-23.502	4.944	16.44	1.00	34.1
626	CD1	LEU	A	898	-22.693	4.872	17.73	1.00	34.32
627	CD2	LEU	A	898	-22.835	5.891	15.452	1.00	34.65
628	N	TYR	A	899	-25.978	3.406	18.342	1.00	29.45
629	CA	TYR	A	899	-27.211	4.037	18.791	1.00	27.41
630	C	TYR	A	899	-26.98	5.521	19.043	1.00	26.03
631	O	TYR	A	899	-26.471	5.92	20.09	1.00	25.27
632	CB	TYR	A	899	-27.722	3.342	20.048	1.00	27.24
633	CG	TYR	A	899	-28.312	1.984	19.753	1.00	28.73
634	CD1	TYR	A	899	-29.692	1.812	19.639	1.00	27.98
635	CD2	TYR	A	899	-27.488	0.875	19.538	1.00	29.09
636	CE1	TYR	A	899	-30.237	0.577	19.318	1.00	28.63
637	CE2	TYR	A	899	-28.024	-0.367	19.214	1.00	28.35
638	CZ	TYR	A	899	-29.398	-0.507	19.105	1.00	29.04
639	OH	TYR	A	899	-29.935	-1.726	18.77	1.00	31.07

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

640	N	LEU	A	900	-27.355	6.332	18.059	1.00	24.02
641	CA	LEU	A	900	-27.183	7.777	18.129	1.00	21.46
642	C	LEU	A	900	-28.328	8.44	18.886	1.00	19.9
643	O	LEU	A	900	-29.492	8.305	18.505	1.00	20.72
644	CB	LEU	A	900	-27.105	8.35	16.71	1.00	21
645	CG	LEU	A	900	-26.828	9.845	16.545	1.00	23.26
646	CD1	LEU	A	900	-25.389	10.166	16.957	1.00	20.58
647	CD2	LEU	A	900	-27.058	10.232	15.092	1.00	23.21
648	N	ALA	A	901	-28	9.148	19.962	1.00	17.46
649	CA	ALA	A	901	-29.021	9.839	20.744	1.00	16.61
650	C	ALA	A	901	-29.198	11.258	20.198	1.00	14.32
651	O	ALA	A	901	-28.224	11.974	19.981	1.00	12.57
652	CB	ALA	A	901	-28.622	9.883	22.224	1.00	16.1
653	N	ILE	A	902	-30.445	11.651	19.968	1.00	13.66
654	CA	ILE	A	902	-30.753	12.98	19.449	1.00	15.26
655	C	ILE	A	902	-31.856	13.63	20.279	1.00	15.62
656	O	ILE	A	902	-32.496	12.97	21.099	1.00	16.98
657	CB	ILE	A	902	-31.226	12.917	17.978	1.00	14.15
658	CG1	ILE	A	902	-32.549	12.155	17.887	1.00	13.15
659	CG2	ILE	A	902	-30.171	12.244	17.125	1.00	14.45
660	CD1	ILE	A	902	-33.162	12.144	16.509	1.00	13.79
661	N	GLU	A	903	-32.086	14.919	20.051	1.00	16.67
662	CA	GLU	A	903	-33.114	15.66	20.782	1.00	17.24
663	C	GLU	A	903	-34.524	15.174	20.484	1.00	16.45
664	O	GLU	A	903	-34.887	14.935	19.333	1.00	16.38
665	CB	GLU	A	903	-33.056	17.154	20.448	1.00	18.43
666	CG	GLU	A	903	-31.88	17.913	21.023	1.00	21.02
667	CD	GLU	A	903	-32.024	19.407	20.815	1.00	22.23
668	OE1	GLU	A	903	-32.049	19.856	19.649	1.00	21
669	OE2	GLU	A	903	-32.124	20.135	21.824	1.00	26.8
670	N	TYR	A	904	-35.321	15.052	21.534	1.00	16.02
671	CA	TYR	A	904	-36.705	14.632	21.396	1.00	17.06
672	C	TYR	A	904	-37.612	15.857	21.26	1.00	17.64
673	O	TYR	A	904	-37.575	16.767	22.093	1.00	17.74
674	CB	TYR	A	904	-37.137	13.82	22.617	1.00	15.31
675	CG	TYR	A	904	-38.629	13.622	22.712	1.00	15.44
676	CD1	TYR	A	904	-39.308	12.828	21.789	1.00	15.33
677	CD2	TYR	A	904	-39.361	14.204	23.745	1.00	15.63
678	CE1	TYR	A	904	-40.675	12.61	21.893	1.00	14.85
679	CE2	TYR	A	904	-40.73	13.992	23.862	1.00	16.91

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

680	CZ	TYR	A	904	-41.382	13.19	22.935	1.00	18.62
681	OH	TYR	A	904	-42.737	12.942	23.075	1.00	22.09
682	N	ALA	A	905	-38.412	15.878	20.198	1.00	18.28
683	CA	ALA	A	905	-39.352	16.968	19.954	1.00	18.47
684	C	ALA	A	905	-40.706	16.552	20.547	1.00	17.86
685	O	ALA	A	905	-41.441	15.752	19.953	1.00	16.38
686	CB	ALA	A	905	-39.478	17.221	18.456	1.00	17.66
687	N	PRO	A	906	-41.051	17.094	21.728	1.00	17.11
688	CA	PRO	A	906	-42.316	16.774	22.411	1.00	17.95
689	C	PRO	A	906	-43.563	17.101	21.593	1.00	18.44
690	O	PRO	A	906	-44.638	16.551	21.841	1.00	18.42
691	CB	PRO	A	906	-42.267	17.627	23.688	1.00	15.89
692	CG	PRO	A	906	-40.812	17.962	23.86	1.00	18.39
693	CD	PRO	A	906	-40.323	18.152	22.445	1.00	17.56
694	N	HIS	A	907	-43.424	17.995	20.621	1.00	16.93
695	CA	HIS	A	907	-44.581	18.394	19.839	1.00	17.57
696	C	HIS	A	907	-44.648	17.913	18.397	1.00	17.02
697	O	HIS	A	907	-45.444	18.421	17.609	1.00	18.86
698	CB	HIS	A	907	-44.709	19.913	19.909	1.00	17.35
699	CG	HIS	A	907	-44.73	20.431	21.312	1.00	17.03
700	ND1	HIS	A	907	-45.825	20.295	22.138	1.00	17.05
701	CD2	HIS	A	907	-43.771	21.033	22.055	1.00	18.79
702	CE1	HIS	A	907	-45.541	20.793	23.328	1.00	18.99
703	NE2	HIS	A	907	-44.3	21.246	23.305	1.00	19.03
704	N	GLY	A	908	-43.829	16.929	18.053	1.00	15.95
705	CA	GLY	A	908	-43.859	16.4	16.699	1.00	16.53
706	C	GLY	A	908	-43.356	17.327	15.605	1.00	17.04
707	O	GLY	A	908	-42.752	18.372	15.879	1.00	17.32
708	N	ASN	A	909	-43.604	16.936	14.356	1.00	16.19
709	CA	ASN	A	909	-43.171	17.721	13.208	1.00	15.96
710	C	ASN	A	909	-44.074	18.936	13.026	1.00	15.28
711	O	ASN	A	909	-45.248	18.913	13.399	1.00	14.72
712	CB	ASN	A	909	-43.154	16.854	11.938	1.00	14.81
713	CG	ASN	A	909	-44.544	16.507	11.44	1.00	16.46
714	OD1	ASN	A	909	-45.144	17.251	10.66	1.00	15.49
715	ND2	ASN	A	909	-45.067	15.372	11.894	1.00	19.51
716	N	LEU	A	910	-43.51	19.995	12.453	1.00	15.71
717	CA	LEU	A	910	-44.226	21.249	12.235	1.00	14.69
718	C	LEU	A	910	-45.467	21.149	11.343	1.00	14.1
719	O	LEU	A	910	-46.422	21.894	11.533	1.00	15.66

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TABLE 3

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

720	CB	LEU	A	910	-43.264	22.289	11.658	1.00	12.64
721	CG	LEU	A	910	-43.825	23.678	11.355	1.00	13.12
722	CD1	LEU	A	910	-44.353	24.331	12.637	1.00	11.41
723	CD2	LEU	A	910	-42.726	24.531	10.739	1.00	10.62
724	N	LEU	A	911	-45.462	20.244	10.37	1.00	12.74
725	CA	LEU	A	911	-46.617	20.128	9.495	1.00	12.56
726	C	LEU	A	911	-47.823	19.673	10.294	1.00	12.75
727	O	LEU	A	911	-48.892	20.276	10.243	1.00	13.86
728	CB	LEU	A	911	-46.353	19.143	8.358	1.00	11.09
729	CG	LEU	A	911	-47.542	18.97	7.408	1.00	7.73
730	CD1	LEU	A	911	-47.885	20.314	6.771	1.00	7.47
731	CD2	LEU	A	911	-47.208	17.935	6.35	1.00	7.42
732	N	ASP	A	912	-47.646	18.599	11.037	1.00	15.59
733	CA	ASP	A	912	-48.722	18.083	11.858	1.00	18.37
734	C	ASP	A	912	-49.151	19.159	12.87	1.00	17.14
735	O	ASP	A	912	-50.345	19.401	13.07	1.00	15.4
736	CB	ASP	A	912	-48.243	16.815	12.566	1.00	23.03
737	CG	ASP	A	912	-49.289	16.227	13.484	1.00	29.3
738	OD1	ASP	A	912	-50.377	15.851	12.993	1.00	34.58
739	OD2	ASP	A	912	-49.02	16.14	14.704	1.00	32.53
740	N	PHE	A	913	-48.175	19.824	13.484	1.00	16.13
741	CA	PHE	A	913	-48.47	20.848	14.475	1.00	15.78
742	C	PHE	A	913	-49.337	21.967	13.883	1.00	16.85
743	O	PHE	A	913	-50.276	22.446	14.528	1.00	16.14
744	CB	PHE	A	913	-47.17	21.43	15.043	1.00	15.22
745	CG	PHE	A	913	-47.352	22.137	16.361	1.00	13.51
746	CD1	PHE	A	913	-47.673	21.417	17.511	1.00	12.93
747	CD2	PHE	A	913	-47.247	23.524	16.446	1.00	13.82
748	CE1	PHE	A	913	-47.893	22.072	18.733	1.00	12.81
749	CE2	PHE	A	913	-47.467	24.194	17.667	1.00	12.61
750	CZ	PHE	A	913	-47.79	23.465	18.806	1.00	12.47
751	N	LEU	A	914	-49.024	22.378	12.654	1.00	15.67
752	CA	LEU	A	914	-49.784	23.425	11.98	1.00	15.79
753	C	LEU	A	914	-51.225	23.003	11.711	1.00	16.13
754	O	LEU	A	914	-52.171	23.749	11.981	1.00	14.89
755	CB	LEU	A	914	-49.121	23.785	10.655	1.00	15.46
756	CG	LEU	A	914	-47.831	24.594	10.757	1.00	15.94
757	CD1	LEU	A	914	-47.231	24.745	9.358	1.00	14.27
758	CD2	LEU	A	914	-48.125	25.956	11.395	1.00	9.15
759	N	ARG	A	915	-51.385	21.803	11.167	1.00	16.27

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

760	CA	ARG	A	915	-52.707	21.281	10.857	1.00	17.5
761	C	ARG	A	915	-53.574	21.055	12.097	1.00	17.86
762	O	ARG	A	915	-54.781	21.306	12.069	1.00	14.9
763	CB	ARG	A	915	-52.563	19.99	10.046	1.00	16.85
764	CG	ARG	A	915	-52.011	20.252	8.656	1.00	15.98
765	CD	ARG	A	915	-51.751	18.991	7.868	1.00	13.8
766	NE	ARG	A	915	-51.415	19.335	6.492	1.00	16.7
767	CZ	ARG	A	915	-51.043	18.464	5.56	1.00	18.26
768	NH1	ARG	A	915	-50.767	18.896	4.335	1.00	16.03
769	NH2	ARG	A	915	-50.938	17.17	5.854	1.00	18.76
770	N	LYS	A	916	-52.962	20.589	13.182	1.00	20.07
771	CA	LYS	A	916	-53.702	20.355	14.423	1.00	22.26
772	C	LYS	A	916	-54.125	21.67	15.066	1.00	21.92
773	O	LYS	A	916	-54.916	21.677	16.007	1.00	22.18
774	CB	LYS	A	916	-52.854	19.579	15.437	1.00	23.23
775	CG	LYS	A	916	-52.654	18.115	15.134	1.00	25.78
776	CD	LYS	A	916	-51.966	17.438	16.308	1.00	30.63
777	CE	LYS	A	916	-51.616	15.995	15.987	1.00	33.84
778	NZ	LYS	A	916	-52.766	15.303	15.348	1.00	36.66
779	N	SER	A	917	-53.587	22.777	14.564	1.00	21.89
780	CA	SER	A	917	-53.906	24.09	15.111	1.00	22.03
781	C	SER	A	917	-55.183	24.673	14.509	1.00	23.69
782	O	SER	A	917	-55.669	25.71	14.975	1.00	24.93
783	CB	SER	A	917	-52.757	25.067	14.855	1.00	23.09
784	OG	SER	A	917	-52.858	25.647	13.559	1.00	19.78
785	N	ARG	A	918	-55.708	24.023	13.467	1.00	22.46
786	CA	ARG	A	918	-56.926	24.476	12.798	1.00	22.48
787	C	ARG	A	918	-58.149	24.174	13.653	1.00	24.27
788	O	ARG	A	918	-58.913	23.241	13.374	1.00	23.69
789	CB	ARG	A	918	-57.071	23.794	11.443	1.00	20.68
790	CG	ARG	A	918	-56.045	24.227	10.428	1.00	16.52
791	CD	ARG	A	918	-56.265	23.506	9.123	1.00	13.27
792	NE	ARG	A	918	-55.332	23.953	8.1	1.00	13.4
793	CZ	ARG	A	918	-55.479	23.722	6.803	1.00	11.65
794	NH1	ARG	A	918	-54.578	24.171	5.947	1.00	15.55
795	NH2	ARG	A	918	-56.534	23.056	6.362	1.00	12.78
796	N	VAL	A	919	-58.32	24.984	14.692	1.00	26.02
797	CA	VAL	A	919	-59.408	24.836	15.641	1.00	27.84
798	C	VAL	A	919	-60.789	25.003	15.004	1.00	29.86
799	O	VAL	A	919	-61.762	24.377	15.431	1.00	29.21

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

800	CB	VAL	A	919	-59.228	25.839	16.797	1.00	28.12
801	CG1	VAL	A	919	-59.407	27.266	16.289	1.00	25.83
802	CG2	VAL	A	919	-60.19	25.51	17.92	1.00	28.98
803	N	LEU	A	920	-60.872	25.832	13.968	1.00	32
804	CA	LEU	A	920	-62.14	26.052	13.281	1.00	33
805	C	LEU	A	920	-62.657	24.716	12.741	1.00	34.13
806	O	LEU	A	920	-63.77	24.623	12.219	1.00	35.87
807	CB	LEU	A	920	-61.949	27.054	12.14	1.00	30.77
808	CG	LEU	A	920	-63.208	27.562	11.439	1.00	28.81
809	CD1	LEU	A	920	-64.126	28.228	12.448	1.00	28.43
810	CD2	LEU	A	920	-62.816	28.541	10.344	1.00	27.44
811	N	GLU	A	921	-61.839	23.681	12.88	1.00	35.26
812	CA	GLU	A	921	-62.206	22.353	12.425	1.00	36.6
813	C	GLU	A	921	-62.092	21.312	13.537	1.00	36.01
814	O	GLU	A	921	-62.878	20.371	13.599	1.00	36.21
815	CB	GLU	A	921	-61.324	21.942	11.257	1.00	38.98
816	CG	GLU	A	921	-61.615	20.55	10.762	1.00	45.04
817	CD	GLU	A	921	-60.758	20.181	9.582	1.00	49.79
818	OE1	GLU	A	921	-60.855	20.866	8.534	1.00	52.47
819	OE2	GLU	A	921	-59.984	19.206	9.706	1.00	52.98
820	N	THR	A	922	-61.116	21.481	14.419	1.00	35.71
821	CA	THR	A	922	-60.925	20.535	15.513	1.00	34.61
822	C	THR	A	922	-61.892	20.815	16.655	1.00	34.35
823	O	THR	A	922	-62.311	19.896	17.358	1.00	36.11
824	CB	THR	A	922	-59.498	20.607	16.062	1.00	33.79
825	OG1	THR	A	922	-59.309	21.863	16.723	1.00	32.47
826	CG2	THR	A	922	-58.49	20.473	14.929	1.00	32.83
827	N	ASP	A	923	-62.232	22.088	16.841	1.00	33.14
828	CA	ASP	A	923	-63.159	22.512	17.89	1.00	30.66
829	C	ASP	A	923	-63.735	23.878	17.531	1.00	28.7
830	O	ASP	A	923	-63.349	24.902	18.098	1.00	28.82
831	CB	ASP	A	923	-62.446	22.581	19.242	1.00	31.92
832	CG	ASP	A	923	-63.366	23.027	20.37	1.00	33.75
833	OD1	ASP	A	923	-64.605	23.028	20.181	1.00	33.6
834	OD2	ASP	A	923	-62.843	23.368	21.454	1.00	35.41
835	N	PRO	A	924	-64.678	23.906	16.578	1.00	26.93
836	CA	PRO	A	924	-65.326	25.136	16.112	1.00	26.74
837	C	PRO	A	924	-65.969	26.017	17.185	1.00	26.13
838	O	PRO	A	924	-66.029	27.237	17.028	1.00	24.53
839	CB	PRO	A	924	-66.331	24.628	15.078	1.00	26.98



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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

840	CG	PRO	A	924	-66.604	23.215	15.526	1.00	26.84
841	CD	PRO	A	924	-65.25	22.724	15.913	1.00	25.12
842	N	ALA	A	925	-66.445	25.413	18.27	1.00	26.53
843	CA	ALA	A	925	-67.058	26.196	19.342	1.00	27.32
844	C	ALA	A	925	-65.998	27.128	19.928	1.00	27.83
845	O	ALA	A	925	-66.24	28.32	20.141	1.00	27.08
846	CB	ALA	A	925	-67.611	25.276	20.423	1.00	26.38
847	N	PHE	A	926	-64.819	26.57	20.18	1.00	28.42
848	CA	PHE	A	926	-63.704	27.338	20.72	1.00	29.89
849	C	PHE	A	926	-63.342	28.45	19.731	1.00	29.67
850	O	PHE	A	926	-63.225	29.624	20.108	1.00	30.66
851	CB	PHE	A	926	-62.49	26.419	20.934	1.00	31.34
852	CG	PHE	A	926	-61.265	27.137	21.431	1.00	33.17
853	CD1	PHE	A	926	-61.186	27.581	22.748	1.00	34.18
854	CD2	PHE	A	926	-60.202	27.394	20.574	1.00	33.34
855	CE1	PHE	A	926	-60.065	28.272	23.205	1.00	35.39
856	CE2	PHE	A	926	-59.077	28.084	21.017	1.00	35.5
857	CZ	PHE	A	926	-59.008	28.525	22.338	1.00	35.27
858	N	ALA	A	927	-63.168	28.066	18.466	1.00	27.27
859	CA	ALA	A	927	-62.823	29.001	17.402	1.00	25.56
860	C	ALA	A	927	-63.808	30.163	17.328	1.00	24.81
861	O	ALA	A	927	-63.406	31.324	17.311	1.00	23.21
862	CB	ALA	A	927	-62.782	28.268	16.06	1.00	25.73
863	N	ILE	A	928	-65.098	29.847	17.274	1.00	25.05
864	CA	ILE	A	928	-66.127	30.881	17.197	1.00	25.58
865	C	ILE	A	928	-66.138	31.746	18.441	1.00	26.1
866	O	ILE	A	928	-66.312	32.96	18.357	1.00	27.43
867	CB	ILE	A	928	-67.537	30.28	17.031	1.00	26.89
868	CG1	ILE	A	928	-67.683	29.657	15.635	1.00	27.63
869	CG2	ILE	A	928	-68.589	31.365	17.257	1.00	25.82
870	CD1	ILE	A	928	-67.586	30.653	14.504	1.00	25.87
871	N	ALA	A	929	-65.95	31.123	19.598	1.00	24.94
872	CA	ALA	A	929	-65.354	31.87	20.843	1.00	25.35
873	C	ALA	A	929	-64.752	32.788	20.932	1.00	26.76
874	O	ALA	A	929	-64.82	33.849	21.552	1.00	27.38
875	CB	ALA	A	929	-65.966	30.921	22.027	1.00	24.61
876	N	ASN	A	930	-63.645	32.386	20.313	1.00	27.09
877	CA	ASN	A	930	-62.439	33.199	20.37	1.00	25.71
878	C	ASN	A	930	-62.134	33.959	19.092	1.00	26.05
879	O	ASN	A	930	-61.087	34.6	18.989	1.00	26.29

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

880	CB	ASN	A	930	-61.253	32.326	20.759	1.00	26.16
881	CG	ASN	A	930	-61.378	31.787	22.167	1.00	27.82
882	OD1	ASN	A	930	-61.18	32.512	23.139	1.00	29.41
883	ND2	ASN	A	930	-61.73	30.513	22.285	1.00	27.96
884	N	SER	A	931	-63.046	33.891	18.124	1.00	24.93
885	CA	SER	A	931	-62.874	34.59	16.852	1.00	24.68
886	C	SER	A	931	-61.538	34.272	16.18	1.00	23.61
887	O	SER	A	931	-60.917	35.142	15.566	1.00	24.2
888	CB	SER	A	931	-62.977	36.108	17.071	1.00	25.04
889	OG	SER	A	931	-64.274	36.484	17.503	1.00	27.03
890	N	THR	A	932	-61.097	33.027	16.284	1.00	22.06
891	CA	THR	A	932	-59.823	32.654	15.691	1.00	22.36
892	C	THR	A	932	-59.902	31.389	14.829	1.00	20.35
893	O	THR	A	932	-60.821	30.583	14.969	1.00	19.36
894	CB	THR	A	932	-58.773	32.441	16.791	1.00	23.01
895	OG1	THR	A	932	-57.483	32.272	16.192	1.00	25.2
896	CG2	THR	A	932	-59.119	31.209	17.616	1.00	20.84
897	N	ALA	A	933	-58.925	31.225	13.943	1.00	18.22
898	CA	ALA	A	933	-58.876	30.068	13.059	1.00	16.68
899	C	ALA	A	933	-57.683	29.172	13.385	1.00	16.5
900	O	ALA	A	933	-57.432	28.191	12.689	1.00	17.57
901	CB	ALA	A	933	-58.803	30.523	11.603	1.00	14.79
902	N	SER	A	934	-56.949	29.513	14.442	1.00	14.54
903	CA	SER	A	934	-55.788	28.728	14.85	1.00	14.82
904	C	SER	A	934	-55.43	28.968	16.317	1.00	15.45
905	O	SER	A	934	-55.687	30.044	16.854	1.00	15.38
906	CB	SER	A	934	-54.578	29.079	13.974	1.00	13.69
907	OG	SER	A	934	-53.439	28.311	14.335	1.00	11.43
908	N	THR	A	935	-54.85	27.964	16.968	1.00	14.99
909	CA	THR	A	935	-54.438	28.131	18.359	1.00	16.23
910	C	THR	A	935	-53.138	28.927	18.342	1.00	16.2
911	O	THR	A	935	-52.649	29.383	19.38	1.00	17.33
912	CB	THR	A	935	-54.17	26.765	19.058	1.00	16.94
913	OG1	THR	A	935	-53.301	25.969	18.24	1.00	15.87
914	CG2	THR	A	935	-55.483	26.014	19.304	1.00	15.73
915	N	LEU	A	936	-52.592	29.089	17.141	1.00	15.79
916	CA	LEU	A	936	-51.34	29.804	16.94	1.00	15.67
917	C	LEU	A	936	-51.567	31.226	16.442	1.00	15.32
918	O	LEU	A	936	-52.383	31.46	15.551	1.00	16.75
919	CB	LEU	A	936	-50.471	29.045	15.928	1.00	13.75

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

920	CG	LEU	A	936	-50.169	27.581	16.247	1.00	14.84
921	CD1	LEU	A	936	-49.493	26.902	15.044	1.00	11.51
922	CD2	LEU	A	936	-49.291	27.512	17.493	1.00	12.64
923	N	SER	A	937	-50.828	32.172	17.009	1.00	14.91
924	CA	SER	A	937	-50.946	33.566	16.607	1.00	13.69
925	C	SER	A	937	-49.967	33.865	15.479	1.00	14.63
926	O	SER	A	937	-49.137	33.031	15.125	1.00	16.63
927	CB	SER	A	937	-50.656	34.493	17.786	1.00	10.76
928	OG	SER	A	937	-49.279	34.486	18.114	1.00	12.67
929	N	SER	A	938	-50.07	35.063	14.919	1.00	16.11
930	CA	SER	A	938	-49.192	35.479	13.839	1.00	18.01
931	C	SER	A	938	-47.738	35.495	14.309	1.00	17.86
932	O	SER	A	938	-46.842	35.018	13.595	1.00	15.74
933	CB	SER	A	938	-49.608	36.868	13.333	1.00	19.3
934	OG	SER	A	938	-48.83	37.26	12.214	1.00	20.25
935	N	GLN	A	939	-47.506	36.041	15.506	1.00	17.98
936	CA	GLN	A	939	-46.148	36.099	16.062	1.00	18.25
937	C	GLN	A	939	-45.546	34.701	16.123	1.00	16.2
938	O	GLN	A	939	-44.441	34.474	15.633	1.00	15.21
939	CB	GLN	A	939	-46.15	36.711	17.475	1.00	18.5
940	CG	GLN	A	939	-46.276	38.229	17.513	1.00	20.34
941	CD	GLN	A	939	-44.976	38.956	17.172	1.00	21.16
942	OE1	GLN	A	939	-44.977	39.911	16.392	1.00	21.28
943	NE2	GLN	A	939	-43.867	38.518	17.772	1.00	18.8
944	N	GLN	A	940	-46.277	33.765	16.723	1.00	15.5
945	CA	GLN	A	940	-45.795	32.391	16.843	1.00	15.71
946	C	GLN	A	940	-45.485	31.782	15.472	1.00	14.46
947	O	GLN	A	940	-44.465	31.117	15.299	1.00	14.21
948	CB	GLN	A	940	-46.817	31.536	17.595	1.00	15.83
949	CG	GLN	A	940	-47.016	31.975	19.038	1.00	18.52
950	CD	GLN	A	940	-47.999	31.095	19.799	1.00	21.31
951	OE1	GLN	A	940	-49.14	30.9	19.371	1.00	22.66
952	NE2	GLN	A	940	-47.562	30.567	20.935	1.00	19.99
953	N	LEU	A	941	-46.357	32.018	14.498	1.00	12.9
954	CA	LEU	A	941	-46.131	31.499	13.156	1.00	11.69
955	C	LEU	A	941	-44.865	32.129	12.575	1.00	11.33
956	O	LEU	A	941	-44.034	31.44	11.987	1.00	10.98
957	CB	LEU	A	941	-47.348	31.782	12.268	1.00	10.17
958	CG	LEU	A	941	-48.614	30.978	12.63	1.00	8.91
959	CD1	LEU	A	941	-49.781	31.432	11.768	1.00	8.02

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

960	CD2	LEU	A	941	-48.374	29.493	12.42	1.00	2.65
961	N	LEU	A	942	-44.697	33.433	12.767	1.00	12.96
962	CA	LEU	A	942	-43.504	34.1	12.257	1.00	12.91
963	C	LEU	A	942	-42.247	33.625	12.961	1.00	13.21
964	O	LEU	A	942	-41.201	33.48	12.329	1.00	13.56
965	CB	LEU	A	942	-43.625	35.619	12.374	1.00	14.59
966	CG	LEU	A	942	-44.469	36.301	11.291	1.00	16.84
967	CD1	LEU	A	942	-44.282	37.815	11.37	1.00	19.33
968	CD2	LEU	A	942	-44.044	35.798	9.916	1.00	17.83
969	N	HIS	A	943	-42.334	33.372	14.265	1.00	12.74
970	CA	HIS	A	943	-41.167	32.881	14.994	1.00	11.95
971	C	HIS	A	943	-40.743	31.503	14.496	1.00	10.33
972	O	HIS	A	943	-39.564	31.162	14.527	1.00	11.63
973	CB	HIS	A	943	-41.44	32.847	16.499	1.00	14.35
974	CG	HIS	A	943	-41.153	34.146	17.183	1.00	17.11
975	ND1	HIS	A	943	-39.899	34.721	17.184	1.00	18.4
976	CD2	HIS	A	943	-41.96	35.001	17.854	1.00	16.48
977	CE1	HIS	A	943	-39.947	35.875	17.823	1.00	17.06
978	NE2	HIS	A	943	-41.186	36.069	18.239	1.00	17.64
979	N	PHE	A	944	-41.701	30.704	14.048	1.00	10.59
980	CA	PHE	A	944	-41.385	29.384	13.502	1.00	11.76
981	C	PHE	A	944	-40.577	29.591	12.222	1.00	10.9
982	O	PHE	A	944	-39.556	28.946	12.02	1.00	10.45
983	CB	PHE	A	944	-42.668	28.608	13.172	1.00	13.64
984	CG	PHE	A	944	-43.299	27.935	14.364	1.00	13.91
985	CD1	PHE	A	944	-44.677	27.764	14.429	1.00	13.91
986	CD2	PHE	A	944	-42.514	27.422	15.388	1.00	13.12
987	CE1	PHE	A	944	-45.259	27.09	15.49	1.00	14.4
988	CE2	PHE	A	944	-43.089	26.745	16.456	1.00	13.54
989	CZ	PHE	A	944	-44.464	26.578	16.506	1.00	14.66
990	N	ALA	A	945	-41.026	30.508	11.366	1.00	9.93
991	CA	ALA	A	945	-40.306	30.767	10.125	1.00	11.63
992	C	ALA	A	945	-38.907	31.305	10.424	1.00	11.3
993	O	ALA	A	945	-37.93	30.896	9.791	1.00	12.83
994	CB	ALA	A	945	-41.087	31.752	9.242	1.00	9.5
995	N	ALA	A	946	-38.818	32.216	11.392	1.00	11.43
996	CA	ALA	A	946	-37.542	32.812	11.799	1.00	11.61
997	C	ALA	A	946	-36.625	31.735	12.37	1.00	12.59
998	O	ALA	A	946	-35.416	31.748	12.129	1.00	13.75
999	CB	ALA	A	946	-37.773	33.905	12.843	1.00	8.68

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## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

1000	N	ASP	A	947	-37.201	30.814	13.137	1.00	13.05
1001	CA	ASP	A	947	-36.433	29.71	13.71	1.00	14.03
1002	C	ASP	A	947	-35.721	28.926	12.604	1.00	13.1
1003	O	ASP	A	947	-34.505	28.743	12.642	1.00	14.39
1004	CB	ASP	A	947	-37.354	28.75	14.476	1.00	15.51
1005	CG	ASP	A	947	-37.657	29.221	15.888	1.00	18.66
1006	OD1	ASP	A	947	-38.566	28.638	16.519	1.00	19.93
1007	OD2	ASP	A	947	-36.985	30.159	16.372	1.00	19
1008	N	VAL	A	948	-36.484	28.464	11.619	1.00	10.46
1009	CA	VAL	A	948	-35.905	27.692	10.532	1.00	10.26
1010	C	VAL	A	948	-34.857	28.516	9.772	1.00	10.96
1011	O	VAL	A	948	-33.791	27.997	9.43	1.00	10.71
1012	CB	VAL	A	948	-37.004	27.191	9.561	1.00	9.72
1013	CG1	VAL	A	948	-36.391	26.289	8.496	1.00	5.45
1014	CG2	VAL	A	948	-38.092	26.452	10.344	1.00	7.16
1015	N	ALA	A	949	-35.151	29.79	9.514	1.00	9.17
1016	CA	ALA	A	949	-34.197	30.659	8.816	1.00	10.34
1017	C	ALA	A	949	-32.895	30.779	9.625	1.00	11.19
1018	O	ALA	A	949	-31.795	30.784	9.058	1.00	11.46
1019	CB	ALA	A	949	-34.808	32.064	8.591	1.00	9.37
1020	N	ARG	A	950	-33.021	30.868	10.949	1.00	8.87
1021	CA	ARG	A	950	-31.851	30.993	11.81	1.00	10.16
1022	C	ARG	A	950	-31.04	29.699	11.773	1.00	10.42
1023	O	ARG	A	950	-29.812	29.727	11.789	1.00	10.5
1024	CB	ARG	A	950	-32.275	31.308	13.258	1.00	11.03
1025	CG	ARG	A	950	-31.123	31.767	14.159	1.00	11.64
1026	CD	ARG	A	950	-31.567	32.058	15.596	1.00	11.08
1027	NE	ARG	A	950	-32.651	33.036	15.643	1.00	12.36
1028	CZ	ARG	A	950	-33.936	32.736	15.828	1.00	13.53
1029	NH1	ARG	A	950	-34.845	33.704	15.841	1.00	12.85
1030	NH2	ARG	A	950	-34.315	31.478	16.019	1.00	10.81
1031	N	GLY	A	951	-31.736	28.567	11.719	1.00	10.75
1032	CA	GLY	A	951	-31.061	27.283	11.677	1.00	10.81
1033	C	GLY	A	951	-30.402	27.043	10.329	1.00	12.86
1034	O	GLY	A	951	-29.312	26.461	10.257	1.00	10.86
1035	N	MET	A	952	-31.05	27.484	9.252	1.00	13.19
1036	CA	MET	A	952	-30.475	27.296	7.918	1.00	14.56
1037	C	MET	A	952	-29.281	28.216	7.673	1.00	14.97
1038	O	MET	A	952	-28.376	27.883	6.904	1.00	15.22
1039	CB	MET	A	952	-31.534	27.5	6.84	1.00	12.78

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

1040	CG	MET	A	952	-32.485	26.318	6.72	1.00	17.29
1041	SD	MET	A	952	-31.591	24.729	6.534	1.00	20.74
1042	CE	MET	A	952	-30.974	24.867	4.849	1.00	15.17
1043	N	ASP	A	953	-29.274	29.37	8.331	1.00	16.69
1044	CA	ASP	A	953	-28.162	30.306	8.197	1.00	15.65
1045	C	ASP	A	953	-26.971	29.601	8.825	1.00	16.75
1046	O	ASP	A	953	-25.891	29.501	8.235	1.00	16.06
1047	CB	ASP	A	953	-28.459	31.595	8.956	1.00	16.13
1048	CG	ASP	A	953	-27.248	32.492	9.074	1.00	15.73
1049	OD1	ASP	A	953	-26.872	32.844	10.211	1.00	20.05
1050	OD2	ASP	A	953	-26.668	32.847	8.034	1.00	15.16
1051	N	TYR	A	954	-27.19	29.093	10.03	1.00	16.18
1052	CA	TYR	A	954	-26.159	28.37	10.748	1.00	15.84
1053	C	TYR	A	954	-25.623	27.191	9.924	1.00	15.57
1054	O	TYR	A	954	-24.411	27.006	9.807	1.00	17.31
1055	CB	TYR	A	954	-26.721	27.857	12.072	1.00	16.2
1056	CG	TYR	A	954	-25.785	26.927	12.802	1.00	17.46
1057	CD1	TYR	A	954	-24.631	27.415	13.43	1.00	17.38
1058	CD2	TYR	A	954	-26.033	25.558	12.841	1.00	14.83
1059	CE1	TYR	A	954	-23.742	26.553	14.08	1.00	18.61
1060	CE2	TYR	A	954	-25.154	24.687	13.486	1.00	18.74
1061	CZ	TYR	A	954	-24.011	25.191	14.1	1.00	19.49
1062	OH	TYR	A	954	-23.136	24.33	14.713	1.00	20.17
1063	N	LEU	A	955	-26.522	26.397	9.349	1.00	14.5
1064	CA	LEU	A	955	-26.109	25.238	8.567	1.00	13.88
1065	C	LEU	A	955	-25.465	25.574	7.226	1.00	14.6
1066	O	LEU	A	955	-24.439	24.993	6.867	1.00	14.19
1067	CB	LEU	A	955	-27.294	24.295	8.341	1.00	13.44
1068	CG	LEU	A	955	-27.828	23.55	9.567	1.00	14.65
1069	CD1	LEU	A	955	-29.04	22.712	9.177	1.00	12.07
1070	CD2	LEU	A	955	-26.736	22.665	10.145	1.00	13.4
1071	N	SER	A	956	-26.058	26.496	6.477	1.00	15.16
1072	CA	SER	A	956	-25.484	26.845	5.185	1.00	17.84
1073	C	SER	A	956	-24.098	27.462	5.363	1.00	18.56
1074	O	SER	A	956	-23.206	27.244	4.542	1.00	18.07
1075	CB	SER	A	956	-26.406	27.805	4.415	1.00	17.34
1076	OG	SER	A	956	-26.596	29.021	5.109	1.00	21.9
1077	N	GLN	A	957	-23.915	28.223	6.439	1.00	20.57
1078	CA	GLN	A	957	-22.625	28.854	6.704	1.00	23.11
1079	C	GLN	A	957	-21.552	27.798	6.918	1.00	22.02

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

1080	O	GLN	A	957	-20.369	28.057	6.735	1.00	20.97
1081	CB	GLN	A	957	-22.709	29.767	7.933	1.00	28.06
1082	CG	GLN	A	957	-23.539	31.022	7.708	1.00	33.83
1083	CD	GLN	A	957	-22.991	31.877	6.583	1.00	38.61
1084	OE1	GLN	A	957	-21.916	32.464	6.703	1.00	41.57
1085	NE2	GLN	A	957	-23.726	31.945	5.477	1.00	40.48
1086	N	LYS	A	958	-21.977	26.606	7.313	1.00	21.81
1087	CA	LYS	A	958	-21.058	25.504	7.528	1.00	21.59
1088	C	LYS	A	958	-21.064	24.587	6.307	1.00	21.98
1089	O	LYS	A	958	-20.727	23.404	6.403	1.00	22.58
1090	CB	LYS	A	958	-21.452	24.722	8.78	1.00	23.72
1091	CG	LYS	A	958	-21.079	25.398	10.092	1.00	23.76
1092	CD	LYS	A	958	-21.78	24.734	11.263	1.00	27.93
1093	CE	LYS	A	958	-21.02	24.939	12.562	1.00	32.13
1094	NZ	LYS	A	958	-19.779	24.104	12.586	1.00	34.41
1095	N	GLN	A	959	-21.465	25.144	5.164	1.00	21.81
1096	CA	GLN	A	959	-21.499	24.421	3.894	1.00	22.48
1097	C	GLN	A	959	-22.59	23.362	3.752	1.00	21.68
1098	O	GLN	A	959	-22.679	22.703	2.718	1.00	23.09
1099	CB	GLN	A	959	-20.139	23.769	3.626	1.00	25.35
1100	CG	GLN	A	959	-18.986	24.74	3.642	1.00	32.08
1101	CD	GLN	A	959	-19.16	25.845	2.615	1.00	38.07
1102	OE1	GLN	A	959	-19.091	25.602	1.405	1.00	41.39
1103	NE2	GLN	A	959	-19.395	27.066	3.091	1.00	39.04
1104	N	PHE	A	960	-23.413	23.189	4.778	1.00	19.77
1105	CA	PHE	A	960	-24.482	22.201	4.713	1.00	19.17
1106	C	PHE	A	960	-25.551	22.53	3.683	1.00	16.96
1107	O	PHE	A	960	-25.965	23.679	3.555	1.00	17.13
1108	CB	PHE	A	960	-25.174	22.05	6.07	1.00	20.48
1109	CG	PHE	A	960	-24.396	21.256	7.063	1.00	21.85
1110	CD1	PHE	A	960	-23.346	21.83	7.765	1.00	23.44
1111	CD2	PHE	A	960	-24.702	19.923	7.287	1.00	23.33
1112	CE1	PHE	A	960	-22.609	21.085	8.678	1.00	23.61
1113	CE2	PHE	A	960	-23.973	19.166	8.198	1.00	24.29
1114	CZ	PHE	A	960	-22.923	19.748	8.897	1.00	22.76
1115	N	ILE	A	961	-25.99	21.506	2.955	1.00	15.18
1116	CA	ILE	A	961	-27.063	21.631	1.967	1.00	13.66
1117	C	ILE	A	961	-28.105	20.605	2.428	1.00	13.57
1118	O	ILE	A	961	-27.805	19.417	2.548	1.00	13.76
1119	CB	ILE	A	961	-26.585	21.285	0.528	1.00	11.69

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## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

1120	CG1	ILE	A	961	-25.451	22.222	0.108	1.00	9.89
1121	CG2	ILE	A	961	-27.736	21.446	-0.461	1.00	9.25
1122	CD1	ILE	A	961	-24.83	21.873	-1.242	1.00	7.7
1123	N	HIS	A	962	-29.324	21.068	2.688	1.00	13.97
1124	CA	HIS	A	962	-30.397	20.21	3.195	1.00	13.97
1125	C	HIS	A	962	-31.06	19.261	2.188	1.00	14.81
1126	O	HIS	A	962	-31.212	18.076	2.467	1.00	16.21
1127	CB	HIS	A	962	-31.457	21.089	3.876	1.00	12.07
1128	CG	HIS	A	962	-32.408	20.324	4.739	1.00	11.42
1129	ND1	HIS	A	962	-33.384	19.498	4.223	1.00	9.39
1130	CD2	HIS	A	962	-32.511	20.235	6.088	1.00	9.35
1131	CE1	HIS	A	962	-34.047	18.934	5.217	1.00	11.44
1132	NE2	HIS	A	962	-33.537	19.363	6.358	1.00	9.44
1133	N	ARG	A	963	-31.465	19.78	1.033	1.00	15.82
1134	CA	ARG	A	963	-32.099	18.977	-0.025	1.00	17.25
1135	C	ARG	A	963	-33.588	18.674	0.16	1.00	17.09
1136	O	ARG	A	963	-34.281	18.361	-0.806	1.00	18.13
1137	CB	ARG	A	963	-31.376	17.626	-0.229	1.00	16.87
1138	CG	ARG	A	963	-29.917	17.68	-0.679	1.00	19.03
1139	CD	ARG	A	963	-29.463	16.299	-1.193	1.00	20.22
1140	NE	ARG	A	963	-30.011	15.213	-0.382	1.00	23.22
1141	CZ	ARG	A	963	-29.591	14.887	0.841	1.00	24.57
1142	NH1	ARG	A	963	-28.591	15.544	1.415	1.00	22.84
1143	NH2	ARG	A	963	-30.211	13.931	1.518	1.00	25
1144	N	ASP	A	964	-34.092	18.74	1.382	1.00	17.77
1145	CA	ASP	A	964	-35.5	18.426	1.586	1.00	18.98
1146	C	ASP	A	964	-36.165	19.309	2.641	1.00	18.42
1147	O	ASP	A	964	-36.866	18.83	3.529	1.00	17.33
1148	CB	ASP	A	964	-35.639	16.939	1.942	1.00	20.47
1149	CG	ASP	A	964	-37.081	16.466	1.933	1.00	24.45
1150	OD1	ASP	A	964	-37.899	17.065	1.206	1.00	25.19
1151	OD2	ASP	A	964	-37.399	15.487	2.645	1.00	28.25
1152	N	LEU	A	965	-35.952	20.611	2.514	1.00	18.21
1153	CA	LEU	A	965	-36.516	21.579	3.44	1.00	19.92
1154	C	LEU	A	965	-38.029	21.674	3.237	1.00	20.24
1155	O	LEU	A	965	-38.496	22.11	2.186	1.00	20.78
1156	CB	LEU	A	965	-35.855	22.941	3.204	1.00	20.02
1157	CG	LEU	A	965	-35.501	23.825	4.398	1.00	21.2
1158	CD1	LEU	A	965	-34.901	22.992	5.543	1.00	20.18
1159	CD2	LEU	A	965	-34.519	24.887	3.924	1.00	17.59



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TABLE 3

STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

1160	N	ALA	A	966	-38.783	21.242	4.244	1.00	19.7
1161	CA	ALA	A	966	-40.242	21.263	4.209	1.00	18.45
1162	C	ALA	A	966	-40.744	21.17	5.644	1.00	18.98
1163	O	ALA	A	966	-40.016	20.707	6.527	1.00	19.06
1164	CB	ALA	A	966	-40.769	20.084	3.397	1.00	18.39
1165	N	ALA	A	967	-41.984	21.594	5.872	1.00	17.44
1166	CA	ALA	A	967	-42.567	21.564	7.21	1.00	16.74
1167	C	ALA	A	967	-42.458	20.2	7.892	1.00	16.65
1168	O	ALA	A	967	-42.289	20.126	9.109	1.00	18.23
1169	CB	ALA	A	967	-44.023	22.002	7.152	1.00	14.31
1170	N	ARG	A	968	-42.552	19.124	7.116	1.00	15.61
1171	CA	ARG	A	968	-42.473	17.775	7.675	1.00	15.8
1172	C	ARG	A	968	-41.094	17.44	8.245	1.00	15.34
1173	O	ARG	A	968	-40.967	16.516	9.054	1.00	14
1174	CB	ARG	A	968	-42.846	16.731	6.613	1.00	15.5
1175	CG	ARG	A	968	-41.955	16.769	5.381	1.00	15.21
1176	CD	ARG	A	968	-42.336	15.713	4.358	1.00	15.14
1177	NE	ARG	A	968	-41.544	15.871	3.145	1.00	16.78
1178	CZ	ARG	A	968	-41.757	16.815	2.235	1.00	19.75
1179	NH1	ARG	A	968	-42.749	17.683	2.388	1.00	24.19
1180	NH2	ARG	A	968	-40.956	16.914	1.188	1.00	21.1
1181	N	ASN	A	969	-40.069	18.178	7.817	1.00	14.31
1182	CA	ASN	A	969	-38.707	17.943	8.303	1.00	13.65
1183	C	ASN	A	969	-38.28	18.934	9.383	1.00	13.7
1184	O	ASN	A	969	-37.092	19.054	9.706	1.00	13.45
1185	CB	ASN	A	969	-37.694	17.954	7.146	1.00	11.94
1186	CG	ASN	A	969	-37.716	16.662	6.338	1.00	13.41
1187	OD1	ASN	A	969	-37.787	15.569	6.9	1.00	12.75
1188	ND2	ASN	A	969	-37.639	16.781	5.018	1.00	11.09
1189	N	ILE	A	970	-39.251	19.661	9.929	1.00	12.04
1190	CA	ILE	A	970	-38.976	20.595	11.009	1.00	11.03
1191	C	ILE	A	970	-39.695	20.034	12.242	1.00	12.81
1192	O	ILE	A	970	-40.829	19.554	12.155	1.00	10.82
1193	CB	ILE	A	970	-39.532	22.01	10.735	1.00	11.34
1194	CG1	ILE	A	970	-38.964	22.578	9.428	1.00	9.96
1195	CG2	ILE	A	970	-39.217	22.916	11.92	1.00	7.07
1196	CD1	ILE	A	970	-37.463	22.778	9.405	1.00	7.62
1197	N	LEU	A	971	-39.037	20.085	13.39	1.00	13.01
1198	CA	LEU	A	971	-39.654	19.582	14.604	1.00	13.92
1199	C	LEU	A	971	-39.907	20.709	15.581	1.00	14.81

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

1200	O	LEU	A	971	-39.18	21.706	15.6	1.00	15.46
1201	CB	LEU	A	971	-38.761	18.512	15.227	1.00	12.61
1202	CG	LEU	A	971	-38.671	17.356	14.226	1.00	15.4
1203	CD1	LEU	A	971	-37.226	17.01	13.962	1.00	16.53
1204	CD2	LEU	A	971	-39.463	16.156	14.741	1.00	13.61
1205	N	VAL	A	972	-40.961	20.558	16.37	1.00	14.66
1206	CA	VAL	A	972	-41.316	21.547	17.377	1.00	14.53
1207	C	VAL	A	972	-40.866	20.963	18.713	1.00	14.99
1208	O	VAL	A	972	-41.475	20.028	19.23	1.00	14.56
1209	CB	VAL	A	972	-42.839	21.794	17.372	1.00	13.61
1210	CG1	VAL	A	972	-43.201	22.887	18.358	1.00	12.55
1211	CG2	VAL	A	972	-43.285	22.181	15.965	1.00	12.89
1212	N	GLY	A	973	-39.783	21.506	19.261	1.00	16.92
1213	CA	GLY	A	973	-39.254	20.984	20.51	1.00	19.45
1214	C	GLY	A	973	-39.694	21.7	21.763	1.00	21.67
1215	O	GLY	A	973	-40.703	22.407	21.76	1.00	22.46
1216	N	GLU	A	974	-38.936	21.502	22.841	1.00	24.24
1217	CA	GLU	A	974	-39.226	22.142	24.121	1.00	26.06
1218	C	GLU	A	974	-39.451	23.629	23.903	1.00	25.33
1219	O	GLU	A	974	-38.847	24.232	23.016	1.00	23.61
1220	CB	GLU	A	974	-38.061	21.974	25.097	1.00	28.52
1221	CG	GLU	A	974	-37.84	20.574	25.623	1.00	35.98
1222	CD	GLU	A	974	-36.751	20.538	26.691	1.00	40.18
1223	OE1	GLU	A	974	-35.609	20.954	26.391	1.00	43.56
1224	OE2	GLU	A	974	-37.034	20.1	27.828	1.00	41.67
1225	N	ASN	A	975	-40.312	24.218	24.725	1.00	25.69
1226	CA	ASN	A	975	-40.614	25.642	24.619	1.00	26.93
1227	C	ASN	A	975	-41.084	25.996	23.21	1.00	23.87
1228	O	ASN	A	975	-41.102	27.159	22.827	1.00	23.59
1229	CB	ASN	A	975	-39.378	26.474	24.978	1.00	30.21
1230	CG	ASN	A	975	-38.916	26.249	26.412	1.00	36.8
1231	OD1	ASN	A	975	-38.546	25.132	26.793	1.00	35.64
1232	ND2	ASN	A	975	-38.932	27.318	27.217	1.00	37.88
1233	N	TYR	A	976	-41.454	24.978	22.443	1.00	22.23
1234	CA	TYR	A	976	-41.934	25.169	21.077	1.00	21.64
1235	C	TYR	A	976	-40.915	25.778	20.114	1.00	20.42
1236	O	TYR	A	976	-41.271	26.566	19.245	1.00	22.04
1237	CB	TYR	A	976	-43.208	26.018	21.086	1.00	20.44
1238	CG	TYR	A	976	-44.352	25.379	21.848	1.00	21.36
1239	CD1	TYR	A	976	-44.512	25.585	23.223	1.00	21.54

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TABLE 3

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

1240	CD2	TYR	A	976	-45.265	24.556	21.196	1.00	21.37
1241	CE1	TYR	A	976	-45.56	24.985	23.928	1.00	21.66
1242	CE2	TYR	A	976	-46.312	23.951	21.884	1.00	22.67
1243	CZ	TYR	A	976	-46.457	24.168	23.245	1.00	23.42
1244	OH	TYR	A	976	-47.497	23.559	23.905	1.00	24.4
1245	N	VAL	A	977	-39.649	25.413	20.272	1.00	19.6
1246	CA	VAL	A	977	-38.597	25.914	19.394	1.00	18.88
1247	C	VAL	A	977	-38.524	24.99	18.175	1.00	18.3
1248	O	VAL	A	977	-38.426	23.773	18.325	1.00	17.82
1249	CB	VAL	A	977	-37.212	25.91	20.11	1.00	19.08
1250	CG1	VAL	A	977	-36.106	26.277	19.126	1.00	16.09
1251	CG2	VAL	A	977	-37.226	26.88	21.295	1.00	15.42
1252	N	ALA	A	978	-38.588	25.567	16.978	1.00	16.81
1253	CA	ALA	A	978	-38.519	24.784	15.747	1.00	16.01
1254	C	ALA	A	978	-37.08	24.32	15.498	1.00	14.99
1255	O	ALA	A	978	-36.141	25.114	15.562	1.00	13.5
1256	CB	ALA	A	978	-39.026	25.612	14.564	1.00	14.35
1257	N	LYS	A	979	-36.918	23.025	15.23	1.00	15.82
1258	CA	LYS	A	979	-35.596	22.438	14.984	1.00	16.1
1259	C	LYS	A	979	-35.556	21.703	13.654	1.00	15.61
1260	O	LYS	A	979	-36.443	20.896	13.358	1.00	16.65
1261	CB	LYS	A	979	-35.234	21.467	16.11	1.00	15.12
1262	CG	LYS	A	979	-35.012	22.149	17.449	1.00	17.05
1263	CD	LYS	A	979	-34.874	21.14	18.585	1.00	18.78
1264	CE	LYS	A	979	-34.484	21.826	19.895	1.00	18.28
1265	NZ	LYS	A	979	-33.116	22.382	19.823	1.00	17.79
1266	N	ILE	A	980	-34.526	21.984	12.859	1.00	13.04
1267	CA	ILE	A	980	-34.366	21.352	11.551	1.00	12.86
1268	C	ILE	A	980	-33.899	19.888	11.616	1.00	13.12
1269	O	ILE	A	980	-32.855	19.587	12.201	1.00	12.43
1270	CB	ILE	A	980	-33.346	22.134	10.675	1.00	12.35
1271	CG1	ILE	A	980	-33.798	23.587	10.516	1.00	11.67
1272	CG2	ILE	A	980	-33.212	21.478	9.296	1.00	8.82
1273	CD1	ILE	A	980	-32.742	24.484	9.879	1.00	10.59
1274	N	ALA	A	981	-34.677	18.981	11.027	1.00	12.2
1275	CA	ALA	A	981	-34.272	17.575	10.986	1.00	12.81
1276	C	ALA	A	981	-33.011	17.625	10.134	1.00	14.28
1277	O	ALA	A	981	-33.045	18.107	8.996	1.00	14.33
1278	CB	ALA	A	981	-35.34	16.715	10.309	1.00	12.6
1279	N	ASP	A	982	-31.906	17.129	10.684	1.00	15.23

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

1280	CA	ASP	A	982	-30.616	17.182	10.01	1.00	16.11
1281	C	ASP	A	982	-29.896	15.856	9.765	1.00	17.68
1282	O	ASP	A	982	-28.66	15.808	9.746	1.00	16.4
1283	CB	ASP	A	982	-29.703	18.116	10.809	1.00	16.13
1284	CG	ASP	A	982	-29.752	17.83	12.302	1.00	17.84
1285	OD1	ASP	A	982	-29.251	18.656	13.088	1.00	17.05
1286	OD2	ASP	A	982	-30.293	16.767	12.687	1.00	19.02
1287	N	PHE	A	983	-30.65	14.779	9.586	1.00	18.33
1288	CA	PHE	A	983	-30.018	13.498	9.32	1.00	18.69
1289	C	PHE	A	983	-29.881	13.349	7.814	1.00	18.59
1290	O	PHE	A	983	-30.773	13.743	7.066	1.00	17.96
1291	CB	PHE	A	983	-30.858	12.333	9.852	1.00	19.28
1292	CG	PHE	A	983	-30.221	10.975	9.628	1.00	18.33
1293	CD1	PHE	A	983	-29.449	10.382	10.621	1.00	19.64
1294	CD2	PHE	A	983	-30.358	10.317	8.408	1.00	16.76
1295	CE1	PHE	A	983	-28.818	9.144	10.401	1.00	20.54
1296	CE2	PHE	A	983	-29.734	9.087	8.174	1.00	15.59
1297	CZ	PHE	A	983	-28.963	8.501	9.172	1.00	18.43
1298	N	GLY	A	984	-28.762	12.784	7.378	1.00	19.5
1299	CA	GLY	A	984	-28.543	12.565	5.959	1.00	18.69
1300	C	GLY	A	984	-28.365	13.803	5.1	1.00	19.44
1301	O	GLY	A	984	-28.726	13.791	3.923	1.00	20.19
1302	N	LEU	A	985	-27.799	14.866	5.664	1.00	18.79
1303	CA	LEU	A	985	-27.598	16.087	4.893	1.00	18.92
1304	C	LEU	A	985	-26.314	16.024	4.075	1.00	19.44
1305	O	LEU	A	985	-25.425	15.209	4.351	1.00	18.88
1306	CB	LEU	A	985	-27.553	17.313	5.815	1.00	18.93
1307	CG	LEU	A	985	-28.745	17.53	6.758	1.00	19.43
1308	CD1	LEU	A	985	-28.722	18.968	7.245	1.00	18.14
1309	CD2	LEU	A	985	-30.065	17.239	6.045	1.00	19.19
1310	N	SER	A	986	-26.234	16.884	3.062	1.00	18.31
1311	CA	SER	A	986	-25.063	16.961	2.2	1.00	18.52
1312	C	SER	A	986	-24.191	18.096	2.69	1.00	18.97
1313	O	SER	A	986	-24.636	18.957	3.448	1.00	17.29
1314	CB	SER	A	986	-25.456	17.244	0.747	1.00	19.08
1315	OG	SER	A	986	-26.197	16.179	0.191	1.00	22.71
1316	N	ARG	A	987	-22.949	18.113	2.232	1.00	20.51
1317	CA	ARG	A	987	-22.032	19.153	2.643	1.00	20.63
1318	C	ARG	A	987	-21.087	19.484	1.494	1.00	19.11
1319	O	ARG	A	987	-20.403	18.617	0.976	1.00	19.26

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

1320	CB	ARG	A	987	-21.272	18.677	3.876	1.00	21.51
1321	CG	ARG	A	987	-20.564	19.772	4.629	1.00	25.19
1322	CD	ARG	A	987	-20.574	19.479	6.113	1.00	25.22
1323	NE	ARG	A	987	-19.82	20.483	6.845	1.00	26.96
1324	CZ	ARG	A	987	-18.497	20.584	6.825	1.00	26.97
1325	NH1	ARG	A	987	-17.775	19.734	6.109	1.00	28.24
1326	NH2	ARG	A	987	-17.897	21.542	7.516	1.00	29.58
1327	N	GLY	A	988	-21.07	20.748	1.092	1.00	19.84
1328	CA	GLY	A	988	-20.214	21.164	-0.001	1.00	18.75
1329	C	GLY	A	988	-20.79	22.353	-0.757	1.00	20.77
1330	O	GLY	A	988	-21.681	23.051	-0.267	1.00	19.87
1331	N	GLN	A	989	-20.274	22.568	-1.962	1.00	20.53
1332	CA	GLN	A	989	-20.682	23.661	-2.831	1.00	20.93
1333	C	GLN	A	989	-22.011	23.365	-3.518	1.00	20.96
1334	O	GLN	A	989	-22.899	24.207	-3.578	1.00	20.73
1335	CB	GLN	A	989	-19.61	23.865	-3.899	1.00	23.27
1336	CG	GLN	A	989	-19.787	25.083	-4.767	1.00	25.62
1337	CD	GLN	A	989	-19.525	26.359	-4.003	1.00	28.58
1338	OE1	GLN	A	989	-18.734	26.378	-3.055	1.00	27.95
1339	NE2	GLN	A	989	-20.172	27.441	-4.42	1.00	32.34
1340	N	GLU	A	990	-22.126	22.155	-4.05	1.00	21.48
1341	CA	GLU	A	990	-23.323	21.733	-4.764	1.00	21.28
1342	C	GLU	A	990	-23.333	20.211	-4.8	1.00	20.33
1343	O	GLU	A	990	-22.276	19.585	-4.756	1.00	20.07
1344	CB	GLU	A	990	-23.281	22.3	-6.181	1.00	22.2
1345	CG	GLU	A	990	-24.347	21.787	-7.125	1.00	25.92
1346	CD	GLU	A	990	-24.175	22.366	-8.515	1.00	27.96
1347	OE1	GLU	A	990	-23.015	22.457	-8.971	1.00	30.16
1348	OE2	GLU	A	990	-25.186	22.724	-9.151	1.00	28.64
1349	N	VAL	A	991	-24.519	19.614	-4.864	1.00	19.2
1350	CA	VAL	A	991	-24.611	18.162	-4.899	1.00	19.84
1351	C	VAL	A	991	-25.622	17.672	-5.923	1.00	20.53
1352	O	VAL	A	991	-26.682	18.258	-6.095	1.00	23.5
1353	CB	VAL	A	991	-24.995	17.587	-3.512	1.00	18.82
1354	CG1	VAL	A	991	-26.37	18.06	-3.114	1.00	18.14
1355	CG2	VAL	A	991	-24.967	16.075	-3.55	1.00	20.15
1356	N	TYR	A	992	-25.277	16.596	-6.613	1.00	21.96
1357	CA	TYR	A	992	-26.166	15.997	-7.598	1.00	22.81
1358	C	TYR	A	992	-26.728	14.725	-6.98	1.00	24.49
1359	O	TYR	A	992	-25.978	13.91	-6.441	1.00	24.68

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

1360	CB	TYR	A	992	-25.399	15.64	-8.868	1.00	22.4
1361	CG	TYR	A	992	-26.14	14.664	-9.756	1.00	24.12
1362	CD1	TYR	A	992	-27.116	15.099	-10.651	1.00	23.74
1363	CD2	TYR	A	992	-25.881	13.296	-9.678	1.00	22.95
1364	CE1	TYR	A	992	-27.811	14.192	-11.444	1.00	25.48
1365	CE2	TYR	A	992	-26.566	12.388	-10.46	1.00	23.97
1366	CZ	TYR	A	992	-27.528	12.835	-11.342	1.00	25.18
1367	OH	TYR	A	992	-28.195	11.92	-12.126	1.00	27.73
1368	N	VAL	A	993	-28.043	14.559	-7.042	1.00	26.66
1369	CA	VAL	A	993	-28.675	13.368	-6.487	1.00	29.76
1370	C	VAL	A	993	-29.747	12.887	-7.458	1.00	33.09
1371	O	VAL	A	993	-30.813	13.494	-7.569	1.00	34.37
1372	CB	VAL	A	993	-29.32	13.659	-5.107	1.00	29.53
1373	CG1	VAL	A	993	-29.806	12.364	-4.471	1.00	27.16
1374	CG2	VAL	A	993	-28.317	14.343	-4.194	1.00	27.79
1375	N	ALA	A	994	-29.449	11.803	-8.17	1.00	36.57
1376	CA	ALA	A	994	-30.372	11.23	-9.148	1.00	39.96
1377	C	ALA	A	994	-31.662	10.748	-8.494	1.00	42.33
1378	O	ALA	A	994	-31.647	10.217	-7.38	1.00	41.55
1379	CB	ALA	A	994	-29.698	10.075	-9.888	1.00	39.92
1380	N	ALA	A	995	-32.776	10.935	-9.197	1.00	45.37
1381	CA	ALA	A	995	-34.086	10.524	-8.696	1.00	49.03
1382	CB	ALA	A	995	-35.173	10.897	-9.709	1.00	48.67
1383	C	ALA	A	995	-34.13	9.022	-8.41	1.00	50.21
1384	OT1	ALA	A	995	-34.394	8.648	-7.243	1.00	51.25
1385	OT2	ALA	A	995	-33.903	8.237	-9.359	1.00	50.97
1386	N	LEU	A	0	-40.171	11.622	-4.283	1.00	34.38
1387	CA	LEU	A	0	-39.478	12.904	-4.614	1.00	34.31
1388	C	LEU	A	0	-40.365	14.112	-4.256	1.00	34.41
1389	O	LEU	A	0	-41.489	14.237	-4.76	1.00	35.79
1390	CB	LEU	A	0	-39.134	12.92	-6.107	1.00	34.57
1391	CG	LEU	A	0	-37.902	13.702	-6.575	1.00	35.72
1392	CD1	LEU	A	0	-36.636	13.129	-5.934	1.00	34.19
1393	CD2	LEU	A	0	-37.808	13.627	-8.092	1.00	34.38
1394	N	PRO	A	1	-39.873	15.012	-3.372	1.00	32.79
1395	CA	PRO	A	1	-40.586	16.219	-2.92	1.00	29.95
1396	C	PRO	A	1	-40.658	17.303	-3.997	1.00	27.35
1397	O	PRO	A	1	-40.229	18.445	-3.796	1.00	26.91
1398	CB	PRO	A	1	-39.773	16.663	-1.707	1.00	30.45
1399	CG	PRO	A	1	-38.38	16.295	-2.102	1.00	30.48

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

1400	CD	PRO	A	1	-38.563	14.905	-2.698	1.00	32.02
1401	N	VAL	A	2	-41.221	16.925	-5.136	1.00	23.63
1402	CA	VAL	A	2	-41.365	17.806	-6.276	1.00	21.18
1403	C	VAL	A	2	-41.93	19.191	-5.961	1.00	20.81
1404	O	VAL	A	2	-41.495	20.191	-6.543	1.00	17.95
1405	CB	VAL	A	2	-42.246	17.12	-7.346	1.00	21.52
1406	CG1	VAL	A	2	-42.578	18.092	-8.482	1.00	19.7
1407	CG2	VAL	A	2	-41.52	15.886	-7.877	1.00	18.09
1408	N	ARG	A	3	-42.888	19.246	-5.04	1.00	19.73
1409	CA	ARG	A	3	-43.541	20.509	-4.673	1.00	19.97
1410	C	ARG	A	3	-42.674	21.546	-3.962	1.00	17.54
1411	O	ARG	A	3	-43.049	22.708	-3.882	1.00	15.85
1412	CB	ARG	A	3	-44.778	20.218	-3.826	1.00	20.26
1413	CG	ARG	A	3	-45.883	19.529	-4.599	1.00	26.96
1414	CD	ARG	A	3	-46.833	18.791	-3.677	1.00	27.25
1415	NE	ARG	A	3	-48.176	18.719	-4.236	1.00	31.55
1416	CZ	ARG	A	3	-48.479	18.131	-5.385	1.00	32.96
1417	NH1	ARG	A	3	-47.53	17.549	-6.106	1.00	34.35
1418	NH2	ARG	A	3	-49.728	18.137	-5.822	1.00	33.46
1419	N	TRP	A	4	-41.521	21.123	-3.455	1.00	15.62
1420	CA	TRP	A	4	-40.617	22.015	-2.741	1.00	14.89
1421	C	TRP	A	4	-39.312	22.253	-3.51	1.00	16.77
1422	O	TRP	A	4	-38.493	23.087	-3.117	1.00	17.13
1423	CB	TRP	A	4	-40.275	21.413	-1.377	1.00	13.84
1424	CG	TRP	A	4	-41.366	21.467	-0.339	1.00	14.71
1425	CD1	TRP	A	4	-41.433	22.321	0.73	1.00	12.88
1426	CD2	TRP	A	4	-42.526	20.623	-0.252	1.00	11.97
1427	NE1	TRP	A	4	-42.557	22.058	1.476	1.00	11.34
1428	CE2	TRP	A	4	-43.247	21.024	0.9	1.00	11.45
1429	CE3	TRP	A	4	-43.026	19.568	-1.03	1.00	11.84
1430	CZ2	TRP	A	4	-44.45	20.403	1.297	1.00	10.05
1431	CZ3	TRP	A	4	-44.227	18.948	-0.635	1.00	10.88
1432	CH2	TRP	A	4	-44.92	19.373	0.522	1.00	9.15
1433	N	MET	A	5	-39.113	21.509	-4.594	1.00	17.2
1434	CA	MET	A	5	-37.895	21.622	-5.389	1.00	17.59
1435	C	MET	A	5	-37.775	22.864	-6.261	1.00	18.54
1436	O	MET	A	5	-38.735	23.293	-6.895	1.00	17.94
1437	CB	MET	A	5	-37.735	20.387	-6.274	1.00	18.52
1438	CG	MET	A	5	-37.213	19.175	-5.541	1.00	19.1
1439	SD	MET	A	5	-37.492	17.67	-6.459	1.00	21.83

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

1440	CE	MET	A	5	-36.327	17.841	-7.826	1.00	15.63
1441	N	ALA	A	6	-36.573	23.427	-6.29	1.00	18.97
1442	CA	ALA	A	6	-36.285	24.599	-7.1	1.00	19.48
1443	C	ALA	A	6	-36.211	24.148	-8.557	1.00	19.78
1444	O	ALA	A	6	-35.905	22.984	-8.838	1.00	20.28
1445	CB	ALA	A	6	-34.949	25.216	-6.664	1.00	17.87
1446	N	ILE	A	7	-36.48	25.065	-9.479	1.00	18.95
1447	CA	ILE	A	7	-36.443	24.747	-10.899	1.00	20.03
1448	C	ILE	A	7	-35.173	24.004	-11.329	1.00	20.36
1449	O	ILE	A	7	-35.249	22.981	-12.008	1.00	19.17
1450	CB	ILE	A	7	-36.596	26.029	-11.746	1.00	21.78
1451	CG1	ILE	A	7	-38.032	26.548	-11.631	1.00	22.76
1452	CG2	ILE	A	7	-36.253	25.749	-13.199	1.00	20.41
1453	CD1	ILE	A	7	-38.295	27.809	-12.444	1.00	26.61
1454	N	GLU	A	8	-34.007	24.514	-10.936	1.00	21
1455	CA	GLU	A	8	-32.752	23.868	-11.307	1.00	20.53
1456	C	GLU	A	8	-32.695	22.437	-10.76	1.00	19.74
1457	O	GLU	A	8	-32.096	21.553	-11.375	1.00	19.3
1458	CB	GLU	A	8	-31.548	24.683	-10.802	1.00	20.26
1459	CG	GLU	A	8	-31.394	24.721	-9.289	1.00	21.21
1460	CD	GLU	A	8	-31.923	26.003	-8.654	1.00	20.76
1461	OE1	GLU	A	8	-32.942	26.558	-9.135	1.00	18.51
1462	OE2	GLU	A	8	-31.32	26.44	-7.652	1.00	20.06
1463	N	SER	A	9	-33.322	22.205	-9.612	1.00	18.03
1464	CA	SER	A	9	-33.333	20.867	-9.03	1.00	19.1
1465	C	SER	A	9	-34.242	19.949	-9.841	1.00	19.43
1466	O	SER	A	9	-33.916	18.788	-10.083	1.00	19.23
1467	CB	SER	A	9	-33.813	20.908	-7.573	1.00	19.52
1468	OG	SER	A	9	-32.872	21.556	-6.729	1.00	18.77
1469	N	LEU	A	10	-35.385	20.474	-10.261	1.00	20.17
1470	CA	LEU	A	10	-36.328	19.691	-11.049	1.00	21.37
1471	C	LEU	A	10	-35.71	19.349	-12.4	1.00	23.02
1472	O	LEU	A	10	-35.867	18.232	-12.895	1.00	23.86
1473	CB	LEU	A	10	-37.627	20.476	-11.269	1.00	19.25
1474	CG	LEU	A	10	-38.506	20.821	-10.065	1.00	17.47
1475	CD1	LEU	A	10	-39.515	21.876	-10.491	1.00	18.53
1476	CD2	LEU	A	10	-39.211	19.579	-9.535	1.00	14.9
1477	N	ASN	A	11	-35.006	20.316	-12.986	1.00	23.39
1478	CA	ASN	A	11	-34.364	20.137	-14.288	1.00	24.75
1479	C	ASN	A	11	-33.094	19.283	-14.301	1.00	25.33



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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

1480	O	ASN	A	11	-32.927	18.432	-15.179	1.00	24.93
1481	CB	ASN	A	11	-34.014	21.497	-14.907	1.00	25.02
1482	CG	ASN	A	11	-35.238	22.274	-15.358	1.00	27.33
1483	OD1	ASN	A	11	-36.296	21.697	-15.601	1.00	29.17
1484	ND2	ASN	A	11	-35.091	23.587	-15.495	1.00	26.17
1485	N	TYR	A	12	-32.201	19.502	-13.333	1.00	25.48
1486	CA	TYR	A	12	-30.933	18.778	-13.321	1.00	23.98
1487	C	TYR	A	12	-30.584	17.962	-12.083	1.00	23.28
1488	O	TYR	A	12	-29.472	17.452	-11.976	1.00	23.79
1489	CB	TYR	A	12	-29.799	19.764	-13.616	1.00	25.23
1490	CG	TYR	A	12	-30.06	20.643	-14.829	1.00	27
1491	CD1	TYR	A	12	-30.342	22.002	-14.685	1.00	26.44
1492	CD2	TYR	A	12	-30.043	20.108	-16.121	1.00	29.08
1493	CE1	TYR	A	12	-30.597	22.81	-15.795	1.00	28.35
1494	CE2	TYR	A	12	-30.3	20.905	-17.243	1.00	30.13
1495	CZ	TYR	A	12	-30.576	22.257	-17.074	1.00	31.38
1496	OH	TYR	A	12	-30.816	23.054	-18.179	1.00	33.15
1497	N	SER	A	13	-31.519	17.834	-11.15	1.00	21.56
1498	CA	SER	A	13	-31.273	17.064	-9.938	1.00	21.75
1499	C	SER	A	13	-30.082	17.505	-9.118	1.00	21.6
1500	O	SER	A	13	-29.411	16.78	-8.433	1.00	21.45
1501	CB	SER	A	13	-31.064	15.579	-10.287	1.00	23.15
1502	OG	SER	A	13	-32.201	15.033	-10.946	1.00	26.14
1503	N	VAL	A	14	-29.815	18.864	-9.181	1.00	20.51
1504	CA	VAL	A	14	-28.708	19.431	-8.416	1.00	20.8
1505	C	VAL	A	14	-29.236	20.239	-7.236	1.00	20.65
1506	O	VAL	A	14	-30.297	20.854	-7.319	1.00	21.18
1507	CB	VAL	A	14	-27.806	20.33	-9.302	1.00	21.18
1508	CG1	VAL	A	14	-27.066	19.473	-10.31	1.00	20.48
1509	CG2	VAL	A	14	-28.641	21.379	-10.018	1.00	19.61
1510	N	TYR	A	15	-28.502	20.228	-6.13	1.00	20.33
1511	CA	TYR	A	15	-28.926	20.965	-4.943	1.00	20.41
1512	C	TYR	A	15	-27.343	21.881	-4.363	1.00	19.5
1513	O	TYR	A	15	-26.677	21.493	-4.24	1.00	18.95
1514	CB	TYR	A	15	-29.406	19.987	-3.863	1.00	19.75
1515	CG	TYR	A	15	-30.517	19.079	-4.33	1.00	19.65
1516	CD1	TYR	A	15	-30.234	17.88	-4.984	1.00	19.66
1517	CD2	TYR	A	15	-31.858	19.441	-4.16	1.00	19.77
1518	CE1	TYR	A	15	-31.26	17.062	-5.466	1.00	21.43
1519	CE2	TYR	A	15	-32.89	18.635	-4.633	1.00	19.25

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

1520	CZ	TYR	A	15	-32.587	17.45	-5.289	1.00	22.07
1521	OH	TYR	A	15	-33.605	16.667	-5.787	1.00	23.1
1522	N	THR	A	16	-28.25	23.095	-4.001	1.00	17.78
1523	CA	THR	A	16	-27.346	24.088	-3.418	1.00	17.3
1524	C	THR	A	16	-28.055	24.825	-2.279	1.00	17.14
1525	O	THR	A	16	-29.198	24.513	-1.944	1.00	16.14
1526	CB	THR	A	16	-26.921	25.135	-4.459	1.00	15.73
1527	OG1	THR	A	16	-28.077	25.865	-4.893	1.00	15.26
1528	CG2	THR	A	16	-26.275	24.465	-5.654	1.00	13.36
1529	N	THR	A	17	-27.371	25.792	-1.676	1.00	16.99
1530	CA	THR	A	17	-27.974	26.574	-0.607	1.00	18.51
1531	C	THR	A	17	-29.085	27.419	-1.214	1.00	18.94
1532	O	THR	A	17	-30.123	27.639	-0.588	1.00	18.89
1533	CB	THR	A	17	-26.947	27.499	0.071	1.00	18.96
1534	OG1	THR	A	17	-26.121	26.718	0.935	1.00	21.5
1535	CG2	THR	A	17	-27.641	28.583	0.897	1.00	19.96
1536	N	ASN	A	18	-28.866	27.88	-2.443	1.00	20.34
1537	CA	ASN	A	18	-29.863	28.686	-3.134	1.00	20.52
1538	C	ASN	A	18	-31.145	27.877	-3.314	1.00	19.74
1539	O	ASN	A	18	-32.24	28.415	-3.166	1.00	21.96
1540	CB	ASN	A	18	-29.34	29.16	-4.498	1.00	22.87
1541	CG	ASN	A	18	-28.229	30.2	-4.375	1.00	25.25
1542	OD1	ASN	A	18	-28.254	31.056	-3.484	1.00	24.36
1543	ND2	ASN	A	18	-27.257	30.141	-5.284	1.00	25.92
1544	N	SER	A	19	-31.023	26.587	-3.619	1.00	17.15
1545	CA	SER	A	19	-32.218	25.77	-3.779	1.00	14.87
1546	C	SER	A	19	-32.884	25.503	-2.428	1.00	15.27
1547	O	SER	A	19	-34.103	25.349	-2.373	1.00	15.23
1548	CB	SER	A	19	-31.908	24.454	-4.505	1.00	14.59
1549	OG	SER	A	19	-30.861	23.717	-3.899	1.00	16.35
1550	N	ASP	A	20	-32.106	25.456	-1.342	1.00	13.39
1551	CA	ASP	A	20	-32.699	25.245	-0.02	1.00	14.97
1552	C	ASP	A	20	-33.6	26.45	0.262	1.00	15.78
1553	O	ASP	A	20	-34.687	26.309	0.838	1.00	15.96
1554	CB	ASP	A	20	-31.642	25.156	1.098	1.00	14.67
1555	CG	ASP	A	20	-30.987	23.783	1.201	1.00	15.78
1556	OD1	ASP	A	20	-31.599	22.77	0.789	1.00	15.61
1557	OD2	ASP	A	20	-29.851	23.718	1.721	1.00	15.46
1558	N	VAL	A	21	-33.146	27.63	-0.158	1.00	13.04
1559	CA	VAL	A	21	-33.912	28.855	0.046	1.00	13.85

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## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

1560	C	VAL	A	21	-35.245	28.8	-0.706	1.00	14.27
1561	O	VAL	A	21	-36.272	29.263	-0.205	1.00	13.94
1562	CB	VAL	A	21	-33.093	30.107	-0.389	1.00	14.08
1563	CG1	VAL	A	21	-34.003	31.326	-0.487	1.00	13.08
1564	CG2	VAL	A	21	-31.972	30.369	0.634	1.00	10.5
1565	N	TRP	A	22	-35.233	28.228	-1.904	1.00	13.88
1566	CA	TRP	A	22	-36.46	28.105	-2.674	1.00	13.75
1567	C	TRP	A	22	-37.415	27.243	-1.859	1.00	13.2
1568	O	TRP	A	22	-38.592	27.566	-1.723	1.00	13.56
1569	CB	TRP	A	22	-36.173	27.451	-4.031	1.00	14.94
1570	CG	TRP	A	22	-37.4	27.093	-4.821	1.00	16.89
1571	CD1	TRP	A	22	-38.364	26.184	-4.478	1.00	16.29
1572	CD2	TRP	A	22	-37.781	27.615	-6.103	1.00	18.42
1573	NE1	TRP	A	22	-39.315	26.106	-5.462	1.00	18.05
1574	CE2	TRP	A	22	-38.985	26.972	-6.473	1.00	19.36
1575	CE3	TRP	A	22	-37.222	28.56	-6.975	1.00	17.64
1576	CZ2	TRP	A	22	-39.643	27.246	-7.682	1.00	18.98
1577	CZ3	TRP	A	22	-37.875	28.833	-8.175	1.00	17.94
1578	CH2	TRP	A	22	-39.075	28.177	-8.516	1.00	18.51
1579	N	SER	A	23	-36.904	28.143	-1.315	1.00	14.15
1580	CA	SER	A	23	-37.719	25.247	-0.494	1.00	15.59
1581	C	SER	A	23	-38.207	25.98	0.754	1.00	15.64
1582	O	SER	A	23	-39.336	25.769	1.207	1.00	16.82
1583	CB	SER	A	23	-36.912	24.02	-0.074	1.00	14.74
1584	OG	SER	A	23	-36.461	23.305	-1.212	1.00	20.83
1585	N	TYR	A	24	-37.354	26.838	1.311	1.00	12.87
1586	CA	TYR	A	24	-37.741	27.602	2.486	1.00	12.67
1587	C	TYR	A	24	-38.978	28.459	2.147	1.00	11.5
1588	O	TYR	A	24	-39.884	28.634	2.971	1.00	9.01
1589	CB	TYR	A	24	-36.589	28.51	2.94	1.00	12.39
1590	CG	TYR	A	24	-36.983	29.367	4.111	1.00	12.22
1591	CD1	TYR	A	24	-36.858	28.891	5.419	1.00	11.18
1592	CD2	TYR	A	24	-37.58	30.615	3.913	1.00	10.88
1593	CE1	TYR	A	24	-37.322	29.626	6.497	1.00	10.73
1594	CE2	TYR	A	24	-38.055	31.365	4.992	1.00	11.52
1595	CZ	TYR	A	24	-37.923	30.863	6.279	1.00	11.24
1596	OH	TYR	A	24	-38.405	31.583	7.349	1.00	10.73
1597	N	GLY	A	25	-38.999	28.99	0.925	1.00	11.06
1598	CA	GLY	A	25	-40.117	29.806	0.484	1.00	9.9
1599	C	GLY	A	25	-41.403	29.01	0.515	1.00	11.09

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

1600	O	GLY	A	25	-42.45	29.521	0.906	1.00	11.07
1601	N	VAL	A	26	-41.323	27.747	0.105	1.00	10.88
1602	CA	VAL	A	26	-42.488	26.881	0.104	1.00	9.56
1603	C	VAL	A	26	-42.831	26.547	1.559	1.00	10.45
1604	O	VAL	A	26	-44.001	26.516	1.941	1.00	9.19
1605	CB	VAL	A	26	-42.214	25.579	-0.697	1.00	10.68
1606	CG1	VAL	A	26	-43.484	24.741	-0.792	1.00	8.08
1607	CG2	VAL	A	26	-41.713	25.925	-2.099	1.00	7.69
1608	N	LEU	A	27	-41.805	26.309	2.373	1.00	11.8
1609	CA	LEU	A	27	-41.999	26	3.791	1.00	11.4
1610	C	LEU	A	27	-42.727	27.17	4.471	1.00	11.99
1611	O	LEU	A	27	-43.68	26.97	5.233	1.00	11.69
1612	CB	LEU	A	27	-40.645	25.754	4.467	1.00	8.97
1613	CG	LEU	A	27	-40.613	25.281	5.929	1.00	11.67
1614	CD1	LEU	A	27	-39.228	24.756	6.231	1.00	13.17
1615	CD2	LEU	A	27	-40.964	26.401	6.893	1.00	9.51
1616	N	LEU	A	28	-42.285	28.39	4.185	1.00	10.98
1617	CA	LEU	A	28	-42.909	29.579	4.766	1.00	11.71
1618	C	LEU	A	28	-44.383	29.648	4.348	1.00	12.55
1619	O	LEU	A	28	-45.257	30.038	5.134	1.00	13.22
1620	CB	LEU	A	28	-42.166	30.842	4.307	1.00	8.88
1621	CG	LEU	A	28	-42.771	32.19	4.711	1.00	10.62
1622	CD1	LEU	A	28	-42.791	32.324	6.217	1.00	9.77
1623	CD2	LEU	A	28	-41.962	33.326	4.088	1.00	12
1624	N	TRP	A	29	-44.644	29.267	3.101	1.00	11.9
1625	CA	TRP	A	29	-45.997	29.255	2.562	1.00	11.29
1626	C	TRP	A	29	-46.824	28.234	3.345	1.00	11.23
1627	O	TRP	A	29	-48.016	28.447	3.581	1.00	9.77
1628	CB	TRP	A	29	-45.966	28.869	1.081	1.00	11.38
1629	CG	TRP	A	29	-47.305	28.911	0.42	1.00	13.41
1630	CD1	TRP	A	29	-47.843	29.956	-0.273	1.00	12.79
1631	CD2	TRP	A	29	-48.28	27.863	0.388	1.00	13.08
1632	NE1	TRP	A	29	-49.088	29.626	-0.737	1.00	14.14
1633	CE2	TRP	A	29	-49.385	28.346	-0.348	1.00	13.55
1634	CE3	TRP	A	29	-48.328	26.562	0.91	1.00	12.5
1635	CZ2	TRP	A	29	-50.528	27.577	-0.58	1.00	11.35
1636	CZ3	TRP	A	29	-49.463	25.797	0.682	1.00	13.46
1637	CH2	TRP	A	29	-50.552	26.312	-0.061	1.00	14
1638	N	GLU	A	30	-46.189	27.122	3.728	1.00	12.06
1639	CA	GLU	A	30	-46.857	26.071	4.509	1.00	12.15

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

1640	C	GLU	A	30	-47.241	26.597	5.893	1.00	13.35
1641	O	GLU	A	30	-48.277	26.217	6.451	1.00	12.78
1642	CB	GLU	A	30	-45.943	24.856	4.721	1.00	11.37
1643	CG	GLU	A	30	-45.633	24.009	3.5	1.00	11.32
1644	CD	GLU	A	30	-44.853	22.766	3.87	1.00	12.46
1645	OE1	GLU	A	30	-45.481	21.7	4.061	1.00	13.01
1646	OE2	GLU	A	30	-43.611	22.858	3.997	1.00	11.55
1647	N	ILE	A	31	-46.38	27.442	6.459	1.00	12.41
1648	CA	ILE	A	31	-46.628	28.004	7.776	1.00	12.84
1649	C	ILE	A	31	-47.781	28.994	7.723	1.00	13.78
1650	O	ILE	A	31	-48.684	28.958	8.564	1.00	13.65
1651	CB	ILE	A	31	-45.371	28.707	8.327	1.00	13.95
1652	CG1	ILE	A	31	-44.323	27.656	8.713	1.00	13.35
1653	CG2	ILE	A	31	-45.734	29.585	9.518	1.00	11.82
1654	CD1	ILE	A	31	-43.002	28.255	9.144	1.00	11.48
1655	N	VAL	A	32	-47.749	29.863	6.719	1.00	13.4
1656	CA	VAL	A	32	-48.778	30.879	6.537	1.00	12.77
1657	C	VAL	A	32	-50.145	30.254	6.284	1.00	13.12
1658	O	VAL	A	32	-51.14	30.66	6.885	1.00	12.7
1659	CB	VAL	A	32	-48.412	31.819	5.356	1.00	12.34
1660	CG1	VAL	A	32	-49.478	32.884	5.176	1.00	12.63
1661	CG2	VAL	A	32	-47.064	32.479	5.626	1.00	12.63
1662	N	SER	A	33	-50.181	29.256	5.401	1.00	13.79
1663	CA	SER	A	33	-51.419	28.568	5.033	1.00	11.96
1664	C	SER	A	33	-51.809	27.5	6.037	1.00	12.22
1665	O	SER	A	33	-52.627	26.625	5.737	1.00	10.33
1666	CB	SER	A	33	-51.271	27.914	3.666	1.00	13.07
1667	OG	SER	A	33	-50.502	26.732	3.771	1.00	17.39
1668	N	LEU	A	34	-51.208	27.566	7.22	1.00	12.43
1669	CA	LEU	A	34	-51.489	26.63	8.304	1.00	12.96
1670	C	LEU	A	34	-51.394	25.147	7.937	1.00	14.01
1671	O	LEU	A	34	-52.225	24.345	8.362	1.00	15.38
1672	CB	LEU	A	34	-52.866	26.929	8.905	1.00	11.4
1673	CG	LEU	A	34	-53.005	28.33	9.527	1.00	14.05
1674	CD1	LEU	A	34	-54.471	28.62	9.828	1.00	12.36
1675	CD2	LEU	A	34	-52.168	28.425	10.806	1.00	8.28
1676	N	GLY	A	35	-50.385	24.785	7.15	1.00	12.83
1677	CA	GLY	A	35	-50.199	23.392	6.793	1.00	12.42
1678	C	GLY	A	35	-50.876	22.883	5.539	1.00	13.43
1679	O	GLY	A	35	-51.081	21.678	5.399	1.00	13.05

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

1680	N	GLY	A	36	-51.217	23.782	4.623	1.00	13.59
1681	CA	GLY	A	36	-51.867	23.356	3.399	1.00	14.71
1682	C	GLY	A	36	-50.913	22.721	2.404	1.00	15.23
1683	O	GLY	A	36	-49.713	22.974	2.421	1.00	16.2
1684	N	THR	A	37	-51.44	21.882	1.524	1.00	17.04
1685	CA	THR	A	37	-50.591	21.234	0.533	1.00	16.32
1686	C	THR	A	37	-50.275	22.218	-0.575	1.00	16.38
1687	O	THR	A	37	-51.183	22.759	-1.202	1.00	19.6
1688	CB	THR	A	37	-51.28	20.016	-0.077	1.00	15.29
1689	OG1	THR	A	37	-51.599	19.088	0.964	1.00	18.05
1690	CG2	THR	A	37	-50.371	19.339	-1.09	1.00	15.48
1691	N	PRO	A	38	-48.981	22.473	-0.825	1.00	16.13
1692	CA	PRO	A	38	-48.54	23.406	-1.874	1.00	15.12
1693	C	PRO	A	38	-49.042	22.97	-3.262	1.00	15
1694	O	PRO	A	38	-48.965	21.791	-3.601	1.00	11.53
1695	CB	PRO	A	38	-47.009	23.337	-1.782	1.00	16.08
1696	CG	PRO	A	38	-46.749	22.87	-0.385	1.00	14.67
1697	CD	PRO	A	38	-47.824	21.853	-0.155	1.00	14.52
1698	N	TYR	A	39	-49.527	23.928	-4.056	1.00	16.36
1699	CA	TYR	A	39	-50.052	23.669	-5.399	1.00	18.48
1700	C	TYR	A	39	-51.167	22.628	-5.3	1.00	22.68
1701	O	TYR	A	39	-51.296	21.767	-6.178	1.00	23
1702	CB	TYR	A	39	-48.962	23.119	-6.337	1.00	16.19
1703	CG	TYR	A	39	-47.67	23.905	-6.395	1.00	12.96
1704	CD1	TYR	A	39	-47.597	25.144	-7.049	1.00	13.63
1705	CD2	TYR	A	39	-46.515	23.411	-5.791	1.00	12.24
1706	CE1	TYR	A	39	-46.392	25.879	-7.094	1.00	9.41
1707	CE2	TYR	A	39	-45.316	24.123	-5.825	1.00	12.11
1708	CZ	TYR	A	39	-45.255	25.356	-6.474	1.00	13.1
1709	OH	TYR	A	39	-44.061	26.052	-6.478	1.00	10.38
1710	N	CYS	A	40	-51.953	22.693	-4.226	1.00	25.61
1711	CA	CYS	A	40	-53.042	21.742	-4.013	1.00	28.27
1712	C	CYS	A	40	-53.896	21.619	-5.269	1.00	29.55
1713	O	CYS	A	40	-54.398	22.614	-5.79	1.00	28.19
1714	CB	CYS	A	40	-53.92	22.182	-2.835	1.00	30.33
1715	SG	CYS	A	40	-54.997	20.868	-2.169	1.00	35.06
1716	N	GLY	A	41	-54.045	20.392	-5.758	1.00	32.07
1717	CA	GLY	A	41	-54.838	20.166	-6.953	1.00	34.06
1718	C	GLY	A	41	-54.019	19.98	-8.22	1.00	35.95
1719	O	GLY	A	41	-54.446	19.275	-9.138	1.00	36.92

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TABLE 3

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

1720	N	MET	A	42	-52.847	20.608	-8.283	1.00	35.64
1721	CA	MET	A	42	-51.988	20.487	-9.457	1.00	34.56
1722	C	MET	A	42	-51.182	19.201	-9.411	1.00	34.44
1723	O	MET	A	42	-50.786	18.743	-8.343	1.00	33.93
1724	CB	MET	A	42	-51.044	21.685	-9.552	1.00	35.17
1725	CG	MET	A	42	-51.754	23.007	-9.76	1.00	35.7
1726	SD	MET	A	42	-50.597	24.364	-9.949	1.00	40.86
1727	CE	MET	A	42	-50.035	24.097	-11.639	1.00	38.18
1728	N	THR	A	43	-50.951	18.612	-10.578	1.00	35.89
1729	CA	THR	A	43	-50.19	17.371	-10.665	1.00	36.37
1730	C	THR	A	43	-48.709	17.696	-10.716	1.00	37.04
1731	O	THR	A	43	-48.325	18.84	-10.974	1.00	36.95
1732	CB	THR	A	43	-50.536	16.587	-11.936	1.00	36.96
1733	OG1	THR	A	43	-50.034	17.294	-13.078	1.00	38.37
1734	CG2	THR	A	43	-52.04	16.429	-12.07	1.00	36.71
1735	N	CYS	A	44	-47.878	16.689	-10.468	1.00	37.18
1736	CA	CYS	A	44	-46.44	16.886	-10.509	1.00	37.49
1737	C	CYS	A	44	-46.041	17.218	-11.939	1.00	37.36
1738	O	CYS	A	44	-45.214	18.097	-12.172	1.00	38.21
1739	CB	CYS	A	44	-45.71	15.631	-10.018	1.00	37.87
1740	SG	CYS	A	44	-45.854	15.341	-8.218	1.00	39.59
1741	N	ALA	A	45	-46.647	16.526	-12.898	1.00	37.27
1742	CA	ALA	A	45	-46.355	16.772	-14.308	1.00	36.92
1743	C	ALA	A	45	-46.622	18.238	-14.654	1.00	36.97
1744	O	ALA	A	45	-45.876	18.848	-15.423	1.00	36.4
1745	CB	ALA	A	45	-47.207	15.862	-15.187	1.00	35.09
1746	N	GLU	A	46	-47.688	18.795	-14.08	1.00	37.32
1747	CA	GLU	A	46	-48.062	20.188	-14.317	1.00	37.7
1748	C	GLU	A	46	-47.04	21.182	-13.771	1.00	37.32
1749	O	GLU	A	46	-46.841	22.254	-14.344	1.00	37.72
1750	CB	GLU	A	46	-49.418	20.49	-13.685	1.00	40.05
1751	CG	GLU	A	46	-50.619	20.022	-14.48	1.00	42.9
1752	CD	GLU	A	46	-51.924	20.371	-13.79	1.00	44.08
1753	OE1	GLU	A	46	-52.206	19.775	-12.726	1.00	44.61
1754	OE2	GLU	A	46	-52.659	21.244	-14.302	1.00	44.34
1755	N	LEU	A	47	-46.404	20.831	-12.658	1.00	36.07
1756	CA	LEU	A	47	-45.411	21.702	-12.043	1.00	34.68
1757	C	LEU	A	47	-44.152	21.79	-12.893	1.00	35.2
1758	O	LEU	A	47	-43.6	22.877	-13.091	1.00	33.22
1759	CB	LEU	A	47	-45.053	21.19	-10.644	1.00	32.6

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

1760	CG	LEU	A	47	-46.166	21.345	-9.613	1.00	30.12
1761	CD1	LEU	A	47	-45.743	20.722	-8.296	1.00	30.63
1762	CD2	LEU	A	47	-46.475	22.821	-9.441	1.00	28.05
1763	N	TYR	A	48	-43.703	20.638	-13.386	1.00	36.28
1764	CA	TYR	A	48	-42.508	20.577	-14.22	1.00	37.23
1765	C	TYR	A	48	-42.671	21.437	-15.454	1.00	37.51
1766	O	TYR	A	48	-41.699	21.945	-15.999	1.00	38.4
1767	CB	TYR	A	48	-42.225	19.141	-14.664	1.00	36.59
1768	CG	TYR	A	48	-41.462	18.308	-13.666	1.00	37.77
1769	CD1	TYR	A	48	-42.122	17.582	-12.674	1.00	38.58
1770	CD2	TYR	A	48	-40.071	18.238	-13.717	1.00	38.62
1771	CE1	TYR	A	48	-41.407	16.8	-11.756	1.00	38.75
1772	CE2	TYR	A	48	-39.348	17.466	-12.808	1.00	38.23
1773	CZ	TYR	A	48	-40.019	16.75	-11.833	1.00	38.77
1774	OH	TYR	A	48	-39.298	15.99	-10.943	1.00	38.88
1775	N	GLU	A	49	-43.913	21.601	-15.887	1.00	39.33
1776	CA	GLU	A	49	-44.208	22.371	-17.084	1.00	41.24
1777	C	GLU	A	49	-44.428	23.858	-16.837	1.00	40.18
1778	O	GLU	A	49	-43.974	24.694	-17.62	1.00	40.3
1779	CB	GLU	A	49	-45.445	21.784	-17.774	1.00	44.62
1780	CG	GLU	A	49	-45.91	22.559	-18.997	1.00	50.11
1781	CD	GLU	A	49	-47.341	22.228	-19.386	1.00	53.49
1782	OE1	GLU	A	49	-48.253	22.454	-18.559	1.00	55.65
1783	OE2	GLU	A	49	-47.557	21.745	-20.518	1.00	56.26
1784	N	LYS	A	50	-45.122	24.19	-15.753	1.00	38.8
1785	CA	LYS	A	50	-45.418	25.588	-15.454	1.00	37.52
1786	C	LYS	A	50	-44.329	26.396	-14.749	1.00	36.4
1787	O	LYS	A	50	-44.04	27.524	-15.155	1.00	36
1788	CB	LYS	A	50	-46.723	25.679	-14.662	1.00	37.33
1789	CG	LYS	A	50	-47.965	25.396	-15.496	1.00	39.07
1790	CD	LYS	A	50	-49.235	25.518	-14.664	1.00	40.01
1791	CE	LYS	A	50	-50.483	25.483	-15.536	1.00	41.81
1792	NZ	LYS	A	50	-50.564	24.249	-16.371	1.00	42.67
1793	N	LEU	A	51	-43.732	25.832	-13.7	1.00	34.89
1794	CA	LEU	A	51	-42.684	26.525	-12.949	1.00	33.12
1795	C	LEU	A	51	-41.625	27.154	-13.858	1.00	33.8
1796	O	LEU	A	51	-41.244	28.308	-13.671	1.00	34.9
1797	CB	LEU	A	51	-42.017	25.561	-11.965	1.00	30.6
1798	CG	LEU	A	51	-42.929	25.01	-10.868	1.00	29.92
1799	CD1	LEU	A	51	-42.242	23.858	-10.166	1.00	29.18



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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

1800	CD2	LEU	A	51	-43.287	26.123	-9.882	1.00	27.13
1801	N	PRO	A	52	-41.131	26.401	-14.854	1.00	34.21
1802	CA	PRO	A	52	-40.115	26.962	-15.752	1.00	34.5
1803	C	PRO	A	52	-40.678	28.119	-16.58	1.00	34.59
1804	O	PRO	A	52	-39.932	28.934	-17.117	1.00	33.31
1805	CB	PRO	A	52	-39.727	25.767	-16.624	1.00	34.55
1806	CG	PRO	A	52	-40.004	24.581	-15.73	1.00	33.86
1807	CD	PRO	A	52	-41.323	24.964	-15.116	1.00	33.79
1808	N	GLN	A	53	-42.004	28.18	-16.667	1.00	35.48
1809	CA	GLN	A	53	-42.684	29.22	-17.424	1.00	36.32
1810	C	GLN	A	53	-43.009	30.449	-16.58	1.00	36.38
1811	O	GLN	A	53	-43.592	31.415	-17.082	1.00	37.07
1812	CB	GLN	A	53	-43.973	28.665	-18.028	1.00	38.91
1813	CG	GLN	A	53	-43.769	27.485	-18.97	1.00	42.74
1814	CD	GLN	A	53	-45.084	26.856	-19.411	1.00	44.9
1815	OE1	GLN	A	53	-45.101	25.912	-20.203	1.00	45.71
1816	NE2	GLN	A	53	-46.193	27.378	-18.893	1.00	44.6
1817	N	GLY	A	54	-42.647	30.413	-15.3	1.00	35.28
1818	CA	GLY	A	54	-42.907	31.552	-14.437	1.00	32.12
1819	C	GLY	A	54	-43.972	31.35	-13.372	1.00	31.19
1820	O	GLY	A	54	-44.089	32.168	-12.459	1.00	30.15
1821	N	TYR	A	55	-44.743	30.27	-13.466	1.00	29.94
1822	CA	TYR	A	55	-45.792	30.022	-12.479	1.00	29.27
1823	C	TYR	A	55	-45.235	29.866	-11.066	1.00	27.66
1824	O	TYR	A	55	-44.221	29.198	-10.854	1.00	26.31
1825	CB	TYR	A	55	-46.613	28.779	-12.849	1.00	29.29
1826	CG	TYR	A	55	-47.757	28.516	-11.893	1.00	29.93
1827	CD1	TYR	A	55	-47.598	27.671	-10.797	1.00	31.54
1828	CD2	TYR	A	55	-48.986	29.154	-12.054	1.00	31.85
1829	CE1	TYR	A	55	-48.629	27.466	-9.882	1.00	31.58
1830	CE2	TYR	A	55	-50.032	28.957	-11.142	1.00	32.53
1831	CZ	TYR	A	55	-49.844	28.11	-10.057	1.00	33.44
1832	OH	TYR	A	55	-50.865	27.902	-9.152	1.00	33.73
1833	N	ARG	A	56	-45.914	30.489	-10.106	1.00	25.51
1834	CA	ARG	A	56	-45.515	30.438	-8.7	1.00	24.39
1835	C	ARG	A	56	-46.762	30.31	-7.815	1.00	23.87
1836	O	ARG	A	56	-47.852	30.738	-8.209	1.00	22.61
1837	CB	ARG	A	56	-44.749	31.717	-8.323	1.00	23.41
1838	CG	ARG	A	56	-43.414	31.922	-9.039	1.00	22.9
1839	CD	ARG	A	56	-42.379	30.864	-8.631	1.00	22.31

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TABLE 3

STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

1840	NE	ARG	A	56	-41.063	31.116	-9.223	1.00	22.12
1841	CZ	ARG	A	56	-40.742	30.855	-10.489	1.00	21.74
1842	NH1	ARG	A	56	-41.643	30.324	-11.308	1.00	19.47
1843	NH2	ARG	A	56	-39.524	31.134	-10.937	1.00	17.57
1844	N	LEU	A	57	-46.602	29.723	-6.628	1.00	22.23
1845	CA	LEU	A	57	-47.721	29.569	-5.697	1.00	21.69
1846	C	LEU	A	57	-48.432	30.907	-5.466	1.00	22.52
1847	O	LEU	A	57	-47.806	31.967	-5.453	1.00	21.78
1848	CB	LEU	A	57	-47.23	29.04	-4.348	1.00	19.98
1849	CG	LEU	A	57	-46.839	27.569	-4.23	1.00	22.53
1850	CD1	LEU	A	57	-45.932	27.367	-3.018	1.00	21.13
1851	CD2	LEU	A	57	-48.101	26.72	-4.13	1.00	19.59
1852	N	GLU	A	58	-49.742	30.856	-5.274	1.00	22.55
1853	CA	GLU	A	58	-50.494	32.072	-5.037	1.00	25.68
1854	C	GLU	A	58	-50.424	32.481	-3.569	1.00	24.19
1855	O	GLU	A	58	-50.187	31.648	-2.695	1.00	22.34
1856	CB	GLU	A	58	-51.938	31.882	-5.505	1.00	29.89
1857	CG	GLU	A	58	-52.028	31.899	-7.034	1.00	38.94
1858	CD	GLU	A	58	-53.226	31.146	-7.585	1.00	44.66
1859	OE1	GLU	A	58	-54.377	31.618	-7.414	1.00	47.07
1860	OE2	GLU	A	58	-53.004	30.074	-8.195	1.00	47.22
1861	N	LYS	A	59	-50.597	33.773	-3.311	1.00	22.6
1862	CA	LYS	A	59	-50.543	34.279	-1.953	1.00	22.36
1863	C	LYS	A	59	-51.728	33.79	-1.147	1.00	21.36
1864	O	LYS	A	59	-52.875	33.936	-1.566	1.00	21.37
1865	CB	LYS	A	59	-50.536	35.805	-1.94	1.00	22.11
1866	CG	LYS	A	59	-50.42	36.38	-0.533	1.00	24.98
1867	CD	LYS	A	59	-50.402	37.903	-0.541	1.00	27.54
1868	CE	LYS	A	59	-51.741	38.472	-0.975	1.00	30.23
1869	NZ	LYS	A	59	-51.695	39.957	-1.08	1.00	34.54
1870	N	PRO	A	60	-51.468	33.183	0.017	1.00	20.33
1871	CA	PRO	A	60	-52.568	32.695	0.851	1.00	19.56
1872	C	PRO	A	60	-53.49	33.87	1.161	1.00	19.6
1873	O	PRO	A	60	-53.051	35.027	1.162	1.00	18.98
1874	CB	PRO	A	60	-51.852	32.17	2.092	1.00	19.93
1875	CG	PRO	A	60	-50.536	31.684	1.525	1.00	19.41
1876	CD	PRO	A	60	-50.161	32.803	0.581	1.00	19.68
1877	N	LEU	A	61	-54.759	33.573	1.42	1.00	18.81
1878	CA	LEU	A	61	-55.747	34.608	1.706	1.00	19.03
1879	C	LEU	A	61	-55.577	35.349	3.033	1.00	18.88

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

1880	O	LEU	A	61	-56.221	36.371	3.262	1.00	22.04
1881	CB	LEU	A	61	-57.151	34.002	1.645	1.00	18.22
1882	CG	LEU	A	61	-57.566	33.41	0.294	1.00	19.86
1883	CD1	LEU	A	61	-58.958	32.796	0.42	1.00	18.36
1884	CD2	LEU	A	61	-57.539	34.498	-0.788	1.00	16.26
1885	N	ASN	A	62	-54.715	34.844	3.902	1.00	17.39
1886	CA	ASN	A	62	-54.5	35.461	5.209	1.00	16.28
1887	C	ASN	A	62	-53.077	35.996	5.307	1.00	15.76
1888	O	ASN	A	62	-52.586	36.297	6.394	1.00	16.76
1889	CB	ASN	A	62	-54.707	34.399	6.286	1.00	15.65
1890	CG	ASN	A	62	-53.663	33.302	6.207	1.00	15.72
1891	OD1	ASN	A	62	-53.234	32.915	5.11	1.00	15.67
1892	ND2	ASN	A	62	-53.247	32.793	7.361	1.00	12.86
1893	N	CYS	A	63	-52.42	36.116	4.161	1.00	16.39
1894	CA	CYS	A	63	-51.035	36.551	4.117	1.00	17.54
1895	C	CYS	A	63	-50.841	38.009	3.725	1.00	17.49
1896	O	CYS	A	63	-51.421	38.472	2.75	1.00	18.08
1897	CB	CYS	A	63	-50.28	35.638	3.149	1.00	17.97
1898	SG	CYS	A	63	-48.505	35.877	3.048	1.00	18.74
1899	N	ASP	A	64	-50.02	38.727	4.493	1.00	18.33
1900	CA	ASP	A	64	-49.732	40.132	4.208	1.00	18.14
1901	C	ASP	A	64	-48.818	40.207	2.99	1.00	17.57
1902	O	ASP	A	64	-47.99	39.331	2.774	1.00	16.16
1903	CB	ASP	A	64	-49.032	40.806	5.393	1.00	18.79
1904	CG	ASP	A	64	-48.778	42.292	5.152	1.00	21.71
1905	OD1	ASP	A	64	-49.695	43.11	5.401	1.00	23.16
1906	OD2	ASP	A	64	-47.667	42.642	4.694	1.00	22.25
1907	N	ASP	A	65	-48.968	41.262	2.201	1.00	19.07
1908	CA	ASP	A	65	-48.155	41.436	1.007	1.00	19.82
1909	C	ASP	A	65	-46.661	41.271	1.243	1.00	19.29
1910	O	ASP	A	65	-45.97	40.697	0.408	1.00	19.45
1911	CB	ASP	A	65	-48.388	42.816	0.38	1.00	22.01
1912	CG	ASP	A	65	-49.714	42.917	-0.341	1.00	25.19
1913	OD1	ASP	A	65	-50.082	41.964	-1.069	1.00	25.79
1914	OD2	ASP	A	65	-50.381	43.961	-0.187	1.00	29
1915	N	GLU	A	66	-46.154	41.776	2.366	1.00	18.35
1916	CA	GLU	A	66	-44.722	41.679	2.617	1.00	18.44
1917	C	GLU	A	66	-44.233	40.247	2.806	1.00	17.8
1918	O	GLU	A	66	-43.167	39.888	2.316	1.00	17.79
1919	CB	GLU	A	66	-44.32	42.519	3.829	1.00	19.55

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TABLE 3

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

1920	CG	GLU	A	66	-42.966	43.172	3.644	1.00	20.61
1921	CD	GLU	A	66	-42.387	43.731	4.929	1.00	22.08
1922	OE1	GLU	A	66	-43.162	44.261	5.75	1.00	19.9
1923	OE2	GLU	A	66	-41.148	43.651	5.105	1.00	21.29
1924	N	VAL	A	67	-45.008	39.427	3.509	1.00	17.2
1925	CA	VAL	A	67	-44.61	38.043	3.722	1.00	16.34
1926	C	VAL	A	67	-44.58	37.326	2.379	1.00	15.72
1927	O	VAL	A	67	-43.644	36.579	2.088	1.00	15.75
1928	CB	VAL	A	67	-45.575	37.301	4.689	1.00	15.96
1929	CG1	VAL	A	67	-45.123	35.863	4.878	1.00	13.83
1930	CG2	VAL	A	67	-45.61	38.006	6.036	1.00	13.95
1931	N	TYR	A	68	-45.593	37.566	1.553	1.00	15.16
1932	CA	TYR	A	68	-45.659	36.928	0.24	1.00	15.88
1933	C	TYR	A	68	-44.483	37.345	-0.639	1.00	16.62
1934	O	TYR	A	68	-43.919	36.528	-1.379	1.00	15.38
1935	CB	TYR	A	68	-46.977	37.275	-0.458	1.00	14.05
1936	CG	TYR	A	68	-47.177	36.569	-1.786	1.00	12.62
1937	CD1	TYR	A	68	-47.137	35.175	-1.872	1.00	10.49
1938	CD2	TYR	A	68	-47.426	37.296	-2.953	1.00	11.29
1939	CE1	TYR	A	68	-47.34	34.519	-3.094	1.00	11.73
1940	CE2	TYR	A	68	-47.633	36.655	-4.178	1.00	12.18
1941	CZ	TYR	A	68	-47.586	35.268	-4.243	1.00	14.42
1942	OH	TYR	A	68	-47.765	34.637	-5.455	1.00	13.81
1943	N	ASP	A	69	-44.117	38.619	-0.551	1.00	17.76
1944	CA	ASP	A	69	-43.002	39.145	-1.324	1.00	20.54
1945	C	ASP	A	69	-41.714	38.417	-0.925	1.00	20.73
1946	O	ASP	A	69	-40.821	38.213	-1.75	1.00	21.86
1947	CB	ASP	A	69	-42.856	40.648	-1.081	1.00	22.99
1948	CG	ASP	A	69	-41.732	41.267	-1.895	1.00	30.5
1949	OD1	ASP	A	69	-41.82	41.261	-3.146	1.00	33.11
1950	OD2	ASP	A	69	-40.752	41.758	-1.287	1.00	34.19
1951	N	LEU	A	70	-41.625	38.03	0.346	1.00	19.29
1952	CA	LEU	A	70	-40.463	37.314	0.851	1.00	16.85
1953	C	LEU	A	70	-40.444	35.939	0.188	1.00	16.41
1954	O	LEU	A	70	-39.394	35.464	-0.248	1.00	15.41
1955	CB	LEU	A	70	-40.555	37.185	2.372	1.00	17
1956	CG	LEU	A	70	-39.454	36.412	3.104	1.00	17.59
1957	CD1	LEU	A	70	-38.097	37.003	2.736	1.00	18.2
1958	CD2	LEU	A	70	-39.676	36.494	4.617	1.00	16.33
1959	N	MET	A	71	-41.609	35.302	0.111	1.00	15.81

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## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

1960	CA	MET	A	71	-41.728	33.996	-0.536	1.00	16.28
1961	C	MET	A	71	-41.276	34.143	-1.988	1.00	16.34
1962	O	MET	A	71	-40.471	33.36	-2.492	1.00	15.38
1963	CB	MET	A	71	-43.186	33.513	-0.558	1.00	16.77
1964	CG	MET	A	71	-43.786	33.104	0.762	1.00	16.66
1965	SD	MET	A	71	-45.541	32.641	0.547	1.00	17.46
1966	CE	MET	A	71	-46.183	33.027	2.203	1.00	15.23
1967	N	ARG	A	72	-41.822	35.152	-2.658	1.00	16.63
1968	CA	ARG	A	72	-41.492	35.404	-4.053	1.00	19.33
1969	C	ARG	A	72	-39.994	35.584	-4.281	1.00	20.28
1970	O	ARG	A	72	-39.464	35.112	-5.288	1.00	20.43
1971	CB	ARG	A	72	-42.266	36.623	-4.567	1.00	19.54
1972	CG	ARG	A	72	-43.779	36.409	-4.594	1.00	22.71
1973	CD	ARG	A	72	-44.136	35.169	-5.401	1.00	22.78
1974	NE	ARG	A	72	-43.743	35.325	-6.803	1.00	25.87
1975	CZ	ARG	A	72	-44.58	35.653	-7.782	1.00	23.87
1976	NH1	ARG	A	72	-45.863	35.852	-7.523	1.00	23.83
1977	NH2	ARG	A	72	-44.13	35.8	-9.016	1.00	25.71
1978	N	GLN	A	73	-39.311	36.261	-3.357	1.00	19.47
1979	CA	GLN	A	73	-37.865	36.45	-3.491	1.00	20.69
1980	C	GLN	A	73	-37.167	35.085	-3.534	1.00	19.79
1981	O	GLN	A	73	-36.254	34.874	-4.333	1.00	20.08
1982	CB	GLN	A	73	-37.295	37.241	-2.308	1.00	22.18
1983	CG	GLN	A	73	-37.757	38.677	-2.181	1.00	26.46
1984	CD	GLN	A	73	-37.25	39.32	-0.89	1.00	30.55
1985	OE1	GLN	A	73	-38.01	39.97	-0.162	1.00	30.97
1986	NE2	GLN	A	73	-35.962	39.138	-0.603	1.00	29.71
1987	N	CYS	A	74	-37.606	34.173	-2.668	1.00	16.31
1988	CA	CYS	A	74	-37.029	32.837	-2.581	1.00	16.47
1989	C	CYS	A	74	-37.21	32.001	-3.842	1.00	16.59
1990	O	CYS	A	74	-36.473	31.035	-4.054	1.00	13.74
1991	CB	CYS	A	74	-37.625	32.073	-1.395	1.00	16.15
1992	SG	CYS	A	74	-37.272	32.789	0.232	1.00	16.15
1993	N	TRP	A	75	-38.183	32.364	-4.676	1.00	16.72
1994	CA	TRP	A	75	-38.42	31.608	-5.899	1.00	17.85
1995	C	TRP	A	75	-38.013	32.328	-7.172	1.00	18.86
1996	O	TRP	A	75	-38.565	32.053	-8.234	1.00	20.21
1997	CB	TRP	A	75	-39.889	31.209	-6.023	1.00	17.87
1998	CG	TRP	A	75	-40.453	30.563	-4.806	1.00	18.53
1999	CD1	TRP	A	75	-39.86	29.604	-4.024	1.00	17.24

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

2000	CD2	TRP	A	75	-41.73	30.823	-4.225	1.00	16.87
2001	NE1	TRP	A	75	-40.695	29.257	-2.99	1.00	15.91
2002	CE2	TRP	A	75	-41.85	29.99	-3.086	1.00	16.61
2003	CE3	TRP	A	75	-42.789	31.681	-4.554	1.00	16.89
2004	CZ2	TRP	A	75	-42.986	29.992	-2.272	1.00	15.12
2005	CZ3	TRP	A	75	-43.924	31.681	-3.743	1.00	17.31
2006	CH2	TRP	A	75	-44.01	30.839	-2.614	1.00	16.8
2007	N	ARG	A	76	-37.07	33.257	-7.074	1.00	19.72
2008	CA	ARG	A	76	-36.611	33.957	-8.265	1.00	23.09
2009	C	ARG	A	76	-35.925	32.921	-9.153	1.00	23.78
2010	O	ARG	A	76	-35.212	32.043	-8.659	1.00	23.49
2011	CB	ARG	A	76	-35.635	35.081	-7.892	1.00	24.75
2012	CG	ARG	A	76	-36.314	36.342	-7.371	1.00	26.75
2013	CD	ARG	A	76	-35.345	37.248	-6.616	1.00	31.18
2014	NE	ARG	A	76	-36.024	38.42	-6.063	1.00	34.35
2015	CZ	ARG	A	76	-35.57	39.151	-5.047	1.00	34.31
2016	NH1	ARG	A	76	-36.273	40.197	-4.624	1.00	34.15
2017	NH2	ARG	A	76	-34.428	38.834	-4.445	1.00	32.4
2018	N	GLU	A	77	-36.146	33.018	-10.459	1.00	25.2
2019	CA	GLU	A	77	-35.563	32.066	-11.398	1.00	27.82
2020	C	GLU	A	77	-34.05	31.881	-11.236	1.00	26.55
2021	O	GLU	A	77	-33.554	30.752	-11.215	1.00	25.44
2022	CB	GLU	A	77	-35.886	32.49	-12.831	1.00	31.28
2023	CG	GLU	A	77	-35.611	31.419	-13.866	1.00	38.7
2024	CD	GLU	A	77	-36.124	31.803	-15.246	1.00	44.96
2025	OE1	GLU	A	77	-37.325	32.146	-15.364	1.00	47.14
2026	OE2	GLU	A	77	-35.331	31.758	-16.214	1.00	47.22
2027	N	LYS	A	78	-33.322	32.985	-11.126	1.00	25.91
2028	CA	LYS	A	78	-31.873	32.927	-10.967	1.00	27.23
2029	C	LYS	A	78	-31.531	32.632	-9.514	1.00	26.48
2030	O	LYS	A	78	-31.759	33.46	-8.631	1.00	27.9
2031	CB	LYS	A	78	-31.249	34.253	-11.403	1.00	28.55
2032	CG	LYS	A	78	-31.581	34.614	-12.844	1.00	31.81
2033	CD	LYS	A	78	-31.021	35.969	-13.21	1.00	35.08
2034	CE	LYS	A	78	-31.368	36.342	-14.633	1.00	36.03
2035	NZ	LYS	A	78	-30.796	37.676	-14.977	1.00	38.67
2036	N	PRO	A	79	-30.963	31.447	-9.248	1.00	25.57
2037	CA	PRO	A	79	-30.601	31.051	-7.885	1.00	25.55
2038	C	PRO	A	79	-29.801	32.112	-7.134	1.00	26.34
2039	O	PRO	A	79	-30.06	32.385	-5.958	1.00	25.37

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

2040	CB	PRO	A	79	-29.797	29.768	-8.1	1.00	24.3
2041	CG	PRO	A	79	-30.352	29.221	-9.381	1.00	24.06
2042	CD	PRO	A	79	-30.471	30.46	-10.226	1.00	25.19
2043	N	TYR	A	80	-28.834	32.709	-7.828	1.00	27.01
2044	CA	TYR	A	80	-27.969	33.719	-7.237	1.00	28.05
2045	C	TYR	A	80	-28.673	35.042	-6.964	1.00	27.88
2046	O	TYR	A	80	-28.074	35.955	-6.406	1.00	28.66
2047	CB	TYR	A	80	-26.739	33.941	-8.127	1.00	30.14
2048	CG	TYR	A	80	-27.066	34.336	-9.55	1.00	32.19
2049	CD1	TYR	A	80	-27.341	35.661	-9.881	1.00	33.41
2050	CD2	TYR	A	80	-27.115	33.381	-10.565	1.00	32.68
2051	CE1	TYR	A	80	-27.655	36.026	-11.189	1.00	34.35
2052	CE2	TYR	A	80	-27.426	33.733	-11.87	1.00	34.24
2053	CZ	TYR	A	80	-27.696	35.058	-12.177	1.00	35.17
2054	OH	TYR	A	80	-28.01	35.413	-13.472	1.00	37.65
2055	N	GLU	A	81	-29.939	35.152	-7.349	1.00	26.98
2056	CA	GLU	A	81	-30.681	36.379	-7.09	1.00	26.82
2057	C	GLU	A	81	-31.594	36.219	-5.875	1.00	25.43
2058	O	GLU	A	81	-32.217	37.18	-5.425	1.00	25.93
2059	CB	GLU	A	81	-31.505	36.791	-8.313	1.00	29.1
2060	CG	GLU	A	81	-30.66	37.208	-9.514	1.00	32.38
2061	CD	GLU	A	81	-31.449	38.011	-10.537	1.00	34.93
2062	OE1	GLU	A	81	-32.506	37.526	-11.001	1.00	35.47
2063	OE2	GLU	A	81	-31.005	39.129	-10.878	1.00	36.45
2064	N	ARG	A	82	-31.662	35.005	-5.338	1.00	21.92
2065	CA	ARG	A	82	-32.495	34.739	-4.17	1.00	20.04
2066	C	ARG	A	82	-31.807	35.252	-2.906	1.00	17.91
2067	O	ARG	A	82	-30.585	35.309	-2.837	1.00	18.84
2068	CB	ARG	A	82	-32.757	33.232	-4.046	1.00	19.07
2069	CG	ARG	A	82	-33.478	32.637	-5.255	1.00	18.07
2070	CD	ARG	A	82	-33.499	31.118	-5.22	1.00	15.31
2071	NE	ARG	A	82	-33.865	30.582	-6.525	1.00	17.5
2072	CZ	ARG	A	82	-33.601	29.345	-6.938	1.00	18.17
2073	NH1	ARG	A	82	-32.965	28.487	-6.145	1.00	14.61
2074	NH2	ARG	A	82	-33.951	28.977	-8.165	1.00	17.02
2075	N	PRO	A	83	-32.585	35.643	-1.889	1.00	16.39
2076	CA	PRO	A	83	-31.938	36.132	-0.672	1.00	16.02
2077	C	PRO	A	83	-31.181	35.028	0.064	1.00	15.96
2078	O	PRO	A	83	-31.331	33.84	-0.231	1.00	15.37
2079	CB	PRO	A	83	-33.109	36.674	0.141	1.00	14.48

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

2080	CG	PRO	A	83	-34.224	35.759	-0.247	1.00	15.19
2081	CD	PRO	A	83	-34.052	35.652	-1.743	1.00	16.2
2082	N	SER	A	84	-30.353	35.435	1.015	1.00	15.96
2083	CA	SER	A	84	-29.592	34.492	1.823	1.00	15.39
2084	C	SER	A	84	-30.423	34.239	3.082	1.00	14.61
2085	O	SER	A	84	-31.236	35.077	3.47	1.00	13.89
2086	CB	SER	A	84	-28.262	35.114	2.232	1.00	14.12
2087	OG	SER	A	84	-28.491	36.155	3.175	1.00	15.97
2088	N	PHE	A	85	-30.218	33.1	3.729	1.00	13.29
2089	CA	PHE	A	85	-30.958	32.815	4.947	1.00	13.84
2090	C	PHE	A	85	-30.785	33.943	5.959	1.00	13.67
2091	O	PHE	A	85	-31.709	34.259	6.709	1.00	14.08
2092	CB	PHE	A	85	-30.51	31.481	5.544	1.00	14.3
2093	CG	PHE	A	85	-31.106	30.287	4.857	1.00	15.35
2094	CD1	PHE	A	85	-32.487	30.059	4.904	1.00	12.95
2095	CD2	PHE	A	85	-30.299	29.399	4.143	1.00	14.51
2096	CE1	PHE	A	85	-33.054	28.956	4.243	1.00	14.44
2097	CE2	PHE	A	85	-30.86	28.291	3.478	1.00	14.34
2098	CZ	PHE	A	85	-32.239	28.073	3.53	1.00	12.65
2099	N	ALA	A	86	-29.61	34.563	5.973	1.00	13.8
2100	CA	ALA	A	86	-29.366	35.679	6.891	1.00	13.89
2101	C	ALA	A	86	-30.286	36.856	6.551	1.00	14.54
2102	O	ALA	A	86	-30.849	37.491	7.447	1.00	16.03
2103	CB	ALA	A	86	-27.894	36.122	6.82	1.00	11.49
2104	N	GLN	A	87	-30.444	37.146	5.26	1.00	14.85
2105	CA	GLN	A	87	-31.306	38.253	4.838	1.00	15.54
2106	C	GLN	A	87	-32.763	37.915	5.112	1.00	15.69
2107	O	GLN	A	87	-33.572	38.799	5.417	1.00	17.32
2108	CB	GLN	A	87	-31.117	38.553	3.346	1.00	16.4
2109	CG	GLN	A	87	-29.693	38.927	2.973	1.00	16.24
2110	CD	GLN	A	87	-29.516	39.108	1.479	1.00	18.62
2111	OE1	GLN	A	87	-29.764	38.186	0.696	1.00	18.55
2112	NE2	GLN	A	87	-29.085	40.301	1.072	1.00	16.07
2113	N	ILE	A	88	-33.101	36.636	5.001	1.00	13.77
2114	CA	ILE	A	88	-34.463	36.203	5.269	1.00	12.92
2115	C	ILE	A	88	-34.757	36.423	6.757	1.00	13.44
2116	O	ILE	A	88	-35.86	36.824	7.123	1.00	14.43
2117	CB	ILE	A	88	-34.659	34.703	4.888	1.00	12.23
2118	CG1	ILE	A	88	-34.606	34.55	3.365	1.00	12.79
2119	CG2	ILE	A	88	-35.995	34.182	5.399	1.00	8.59



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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

2120	CD1	ILE	A	88	-34.793	33.121	2.884	1.00	13.71
2121	N	LEU	A	89	-33.765	36.181	7.609	1.00	12.06
2122	CA	LEU	A	89	-33.943	36.354	9.049	1.00	13.93
2123	C	LEU	A	89	-34.104	37.83	9.432	1.00	15.58
2124	O	LEU	A	89	-34.888	38.168	10.329	1.00	13.73
2125	CB	LEU	A	89	-32.756	35.749	9.801	1.00	13.78
2126	CG	LEU	A	89	-32.841	35.726	11.328	1.00	16.21
2127	CD1	LEU	A	89	-34.067	34.928	11.785	1.00	15.11
2128	CD2	LEU	A	89	-31.56	35.107	11.878	1.00	14.3
2129	N	VAL	A	90	-33.363	38.704	8.752	1.00	15.06
2130	CA	VAL	A	90	-33.445	40.137	9.013	1.00	15.23
2131	C	VAL	A	90	-34.842	40.647	8.667	1.00	16.56
2132	O	VAL	A	90	-35.412	41.453	9.397	1.00	15.43
2133	CB	VAL	A	90	-32.375	40.926	8.19	1.00	16.64
2134	CG1	VAL	A	90	-32.757	42.406	8.085	1.00	12.67
2135	CG2	VAL	A	90	-31.005	40.788	8.859	1.00	10.25
2136	N	SER	A	91	-35.404	40.162	7.564	1.00	16.53
2137	CA	SER	A	91	-36.74	40.592	7.156	1.00	16.13
2138	C	SER	A	91	-37.786	40.142	8.169	1.00	17.19
2139	O	SER	A	91	-38.65	40.922	8.572	1.00	18.89
2140	CB	SER	A	91	-37.096	40.014	5.789	1.00	14.32
2141	OG	SER	A	91	-36.078	40.277	4.846	1.00	18.54
2142	N	LEU	A	92	-37.713	38.877	8.573	1.00	16.15
2143	CA	LEU	A	92	-38.674	38.338	9.533	1.00	14.94
2144	C	LEU	A	92	-38.562	39.019	10.895	1.00	15.24
2145	O	LEU	A	92	-39.573	39.268	11.553	1.00	13.95
2146	CB	LEU	A	92	-38.482	36.822	9.685	1.00	13.55
2147	CG	LEU	A	92	-38.682	36.028	8.394	1.00	12.04
2148	CD1	LEU	A	92	-38.259	34.575	8.599	1.00	10.08
2149	CD2	LEU	A	92	-40.145	36.128	7.971	1.00	11.29
2150	N	ASN	A	93	-37.342	39.331	11.323	1.00	15.65
2151	CA	ASN	A	93	-37.183	39.986	12.613	1.00	17.08
2152	C	ASN	A	93	-37.758	41.398	12.616	1.00	17.73
2153	O	ASN	A	93	-38.228	41.873	13.653	1.00	17.27
2154	CB	ASN	A	93	-35.713	40.019	13.038	1.00	17.07
2155	CG	ASN	A	93	-35.23	38.679	13.552	1.00	18.53
2156	OD1	ASN	A	93	-36.02	37.879	14.051	1.00	19.71
2157	ND2	ASN	A	93	-33.932	38.432	13.449	1.00	19.09
2158	N	ARG	A	94	-37.738	42.063	11.461	1.00	17.32
2159	CA	ARG	A	94	-38.266	43.419	11.378	1.00	19.55

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

2160	C	ARG	A	94	-39.785	43.367	11.506	1.00	21.53
2161	O	ARG	A	94	-40.386	44.201	12.195	1.00	22.24
2162	CB	ARG	A	94	-37.846	44.093	10.058	1.00	19.15
2163	CG	ARG	A	94	-36.37	43.875	9.739	1.00	20.98
2164	CD	ARG	A	94	-35.531	45.126	9.516	1.00	20.6
2165	NE	ARG	A	94	-35.585	45.594	8.133	1.00	20.87
2166	CZ	ARG	A	94	-34.631	46.308	7.539	1.00	18.84
2167	NH1	ARG	A	94	-33.529	46.645	8.198	1.00	17.54
2168	NH2	ARG	A	94	-34.782	46.685	6.277	1.00	18.42
2169	N	MET	A	95	-40.407	42.38	10.865	1.00	21.76
2170	CA	MET	A	95	-41.86	42.241	10.946	1.00	21.33
2171	C	MET	A	95	-42.266	41.839	12.357	1.00	21.26
2172	O	MET	A	95	-43.27	42.325	12.883	1.00	21.67
2173	CB	MET	A	95	-42.372	41.206	9.934	1.00	21.15
2174	CG	MET	A	95	-42.258	41.653	8.479	1.00	22.5
2175	SD	MET	A	95	-42.952	40.459	7.308	1.00	25.43
2176	CE	MET	A	95	-41.512	39.521	6.848	1.00	21.28
2177	N	LEU	A	96	-41.474	40.967	12.975	1.00	21.16
2178	CA	LEU	A	96	-41.752	40.505	14.333	1.00	22.39
2179	C	LEU	A	96	-41.713	41.636	15.356	1.00	24.44
2180	O	LEU	A	96	-42.506	41.662	16.293	1.00	24.22
2181	CB	LEU	A	96	-40.75	39.424	14.746	1.00	19.77
2182	CG	LEU	A	96	-40.978	38.016	14.186	1.00	19.29
2183	CD1	LEU	A	96	-39.729	37.181	14.403	1.00	15.59
2184	CD2	LEU	A	96	-42.201	37.376	14.849	1.00	16.08
2185	N	GLU	A	97	-40.8	42.579	15.161	1.00	27.92
2186	CA	GLU	A	97	-40.646	43.693	16.084	1.00	30.9
2187	C	GLU	A	97	-41.775	44.73	16.026	1.00	31.92
2188	O	GLU	A	97	-41.869	45.596	16.894	1.00	32.14
2189	CB	GLU	A	97	-39.297	44.366	15.829	1.00	33.79
2190	CG	GLU	A	97	-38.903	45.416	16.849	1.00	40.46
2191	CD	GLU	A	97	-38.863	44.869	18.272	1.00	44.52
2192	OE1	GLU	A	97	-38.413	43.713	18.459	1.00	44.18
2193	OE2	GLU	A	97	-39.273	45.608	19.198	1.00	44.69
2194	N	GLU	A	98	-42.637	44.645	15.018	1.00	32.21
2195	CA	GLU	A	98	-43.737	45.602	14.894	1.00	32.86
2196	C	GLU	A	98	-45.038	45.069	15.492	1.00	33.48
2197	O	GLU	A	98	-45.204	43.862	15.671	1.00	35.65
2198	CB	GLU	A	98	-43.943	45.967	13.417	1.00	32.23
2199	CG	GLU	A	98	-42.669	46.492	12.75	1.00	32.85

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## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

2200	CD	GLU	A	98	-42.787	46.658	11.243	1.00	33.92
2201	OE1	GLU	A	98	-43.414	45.805	10.58	1.00	34.64
2202	OE2	GLU	A	98	-42.229	47.635	10.711	1.00	33.97
2203	N	ALA	A	99	-45.959	45.97	15.814	1.00	33.8
2204	CA	ALA	A	99	-47.245	45.572	16.382	1.00	34.41
2205	C	ALA	A	99	-48.065	44.838	15.327	1.00	35.1
2206	O	ALA	A	99	-48.575	43.742	15.571	1.00	37.2
2207	CB	ALA	A	99	-48.008	46.797	16.872	1.00	32.66
2208	N	LYS	A	100	-48.168	45.453	14.152	1.00	33.92
2209	CA	LYS	A	100	-48.922	44.915	13.022	1.00	32.64
2210	C	LYS	A	100	-48.936	43.39	12.898	1.00	31.41
2211	O	LYS	A	100	-47.958	42.713	13.224	1.00	30.88
2212	CB	LYS	A	100	-48.39	45.523	11.719	1.00	33.64
2213	CG	LYS	A	100	-49.142	45.078	10.472	1.00	34.65
2214	CD	LYS	A	100	-48.607	45.752	9.21	1.00	34.73
2215	CE	LYS	A	100	-49.406	45.309	7.994	1.00	33.83
2216	NZ	LYS	A	100	-48.946	45.963	6.741	1.00	36.88
2217	N	THR	A	101	-50.07	42.869	12.434	1.00	29.3
2218	CA	THR	A	101	-50.267	41.441	12.219	1.00	27.29
2219	C	THR	A	101	-49.891	41.15	10.761	1.00	27.47
2220	O	THR	A	101	-50.353	41.843	9.847	1.00	26.72
2221	CB	THR	A	101	-51.74	41.046	12.427	1.00	26.46
2222	OG1	THR	A	101	-52.095	41.228	13.8	1.00	27.46
2223	CG2	THR	A	101	-51.972	39.594	12.037	1.00	27.87
2224	N	TYR	A	102	-49.059	40.135	10.539	1.00	24.39
2225	CA	TYR	A	102	-48.645	39.799	9.184	1.00	23.05
2226	C	TYR	A	102	-49.266	38.521	8.646	1.00	20.98
2227	O	TYR	A	102	-49.464	38.386	7.443	1.00	20.54
2228	CB	TYR	A	102	-47.119	39.73	9.097	1.00	23.19
2229	CG	TYR	A	102	-46.501	41.1	9.054	1.00	24.64
2230	CD1	TYR	A	102	-46.14	41.769	10.228	1.00	25.69
2231	CD2	TYR	A	102	-46.349	41.768	7.841	1.00	24.47
2232	CE1	TYR	A	102	-45.648	43.075	10.187	1.00	24.94
2233	CE2	TYR	A	102	-45.86	43.068	7.789	1.00	24.57
2234	CZ	TYR	A	102	-45.513	43.717	8.961	1.00	25.38
2235	OH	TYR	A	102	-45.038	45.008	8.896	1.00	26.28
2236	N	VAL	A	103	-49.57	37.589	9.542	1.00	19.46
2237	CA	VAL	A	103	-50.197	36.33	9.164	1.00	19.12
2238	C	VAL	A	103	-51.483	36.241	9.976	1.00	19.99
2239	O	VAL	A	103	-51.467	35.85	11.147	1.00	21.47

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

2240	CB	VAL	A	103	-49.284	35.122	9.484	1.00	18.1
2241	CG1	VAL	A	103	-49.99	33.835	9.114	1.00	17.27
2242	CG2	VAL	A	103	-47.971	35.237	8.711	1.00	15.34
2243	N	ASN	A	104	-52.595	36.612	9.348	1.00	19.81
2244	CA	ASN	A	104	-53.897	36.632	10.008	1.00	20.52
2245	C	ASN	A	104	-54.508	35.291	10.423	1.00	20.81
2246	O	ASN	A	104	-54.468	34.309	9.676	1.00	19.61
2247	CB	ASN	A	104	-54.903	37.379	9.132	1.00	20.68
2248	CG	ASN	A	104	-56.285	37.422	9.752	1.00	23.04
2249	OD1	ASN	A	104	-56.486	38.03	10.804	1.00	21.81
2250	ND2	ASN	A	104	-57.245	36.762	9.109	1.00	24.59
2251	N	THR	A	105	-55.089	35.273	11.62	1.00	20.06
2252	CA	THR	A	105	-55.749	34.086	12.157	1.00	21.57
2253	C	THR	A	105	-57.08	34.487	12.785	1.00	21.62
2254	O	THR	A	105	-57.745	33.688	13.444	1.00	22.67
2255	CB	THR	A	105	-54.901	33.39	13.235	1.00	21.86
2256	OG1	THR	A	105	-54.644	34.311	14.3	1.00	23.93
2257	CG2	THR	A	105	-53.59	32.888	12.649	1.00	21.83
2258	N	THR	A	106	-57.468	35.739	12.578	1.00	22.52
2259	CA	THR	A	106	-58.722	36.237	13.116	1.00	20.74
2260	C	THR	A	106	-59.797	35.948	12.078	1.00	20.85
2261	O	THR	A	106	-59.574	36.11	10.874	1.00	19.58
2262	CB	THR	A	106	-58.628	37.741	13.378	1.00	21.51
2263	OG1	THR	A	106	-57.385	38.017	14.033	1.00	22.74
2264	CG2	THR	A	106	-59.775	38.207	14.265	1.00	19.69
2265	N	LEU	A	107	-60.961	35.514	12.543	1.00	20.25
2266	CA	LEU	A	107	-62.046	35.174	11.636	1.00	21.13
2267	C	LEU	A	107	-62.643	36.355	10.889	1.00	22.5
2268	O	LEU	A	107	-62.821	36.299	9.67	1.00	20.79
2269	CB	LEU	A	107	-63.158	34.435	12.393	1.00	18.13
2270	CG	LEU	A	107	-62.75	33.085	12.988	1.00	17.43
2271	CD1	LEU	A	107	-63.975	32.377	13.548	1.00	17.76
2272	CD2	LEU	A	107	-62.095	32.229	11.918	1.00	15.76
2273	N	TYR	A	108	-62.937	37.427	11.623	1.00	25
2274	CA	TYR	A	108	-63.554	38.609	11.036	1.00	25.41
2275	C	TYR	A	108	-64.841	38.169	10.349	1.00	26.07
2276	O	TYR	A	108	-65.689	37.54	10.979	1.00	25.75
2277	CB	TYR	A	108	-62.598	39.289	10.045	1.00	26.12
2278	CG	TYR	A	108	-61.424	39.972	10.721	1.00	27.36
2279	CD1	TYR	A	108	-60.113	39.708	10.326	1.00	26.47

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## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

2280	CD2	TYR	A	108	-61.623	40.87	11.778	1.00	28.27
2281	CE1	TYR	A	108	-59.034	40.31	10.965	1.00	25.91
2282	CE2	TYR	A	108	-60.547	41.477	12.422	1.00	27.23
2283	CZ	TYR	A	108	-59.258	41.188	12.011	1.00	26.76
2284	OH	TYR	A	108	-58.191	41.751	12.665	1.00	27.31
2285	N	GLU	A	109	-64.988	38.467	9.063	1.00	27.42
2286	CA	GLU	A	109	-66.21	38.094	8.361	1.00	30.26
2287	C	GLU	A	109	-66.073	36.907	7.424	1.00	29.17
2288	O	GLU	A	109	-67.071	36.383	6.922	1.00	28.09
2289	CB	GLU	A	109	-66.758	39.299	7.596	1.00	34.38
2290	CG	GLU	A	109	-67.15	40.447	8.513	1.00	40.55
2291	CD	GLU	A	109	-68.175	41.365	7.89	1.00	44.89
2292	OE1	GLU	A	109	-68.651	42.285	8.592	1.00	48.58
2293	OE2	GLU	A	109	-68.506	41.167	6.699	1.00	47.78
2294	N	LYS	A	110	-64.84	36.474	7.199	1.00	28.13
2295	CA	LYS	A	110	-64.597	35.344	6.321	1.00	27.74
2296	C	LYS	A	110	-63.176	34.822	6.439	1.00	26.26
2297	O	LYS	A	110	-62.215	35.591	6.371	1.00	27.44
2298	CB	LYS	A	110	-64.877	35.741	4.866	1.00	29.65
2299	CG	LYS	A	110	-64.587	34.646	3.853	1.00	32.62
2300	CD	LYS	A	110	-65.072	35.013	2.457	1.00	33.94
2301	CE	LYS	A	110	-64.788	33.881	1.475	1.00	36.94
2302	NZ	LYS	A	110	-65.371	34.114	0.116	1.00	39.63
2303	N	PHE	A	111	-63.048	33.513	6.629	1.00	23
2304	CA	PHE	A	111	-61.74	32.888	6.712	1.00	20.34
2305	C	PHE	A	111	-61.768	31.544	6.001	1.00	19.59
2306	O	PHE	A	111	-62.702	30.752	6.152	1.00	17.46
2307	CB	PHE	A	111	-61.289	32.712	8.161	1.00	18.89
2308	CG	PHE	A	111	-59.842	32.32	8.289	1.00	19.73
2309	CD1	PHE	A	111	-59.411	31.05	7.908	1.00	19.52
2310	CD2	PHE	A	111	-58.9	33.234	8.754	1.00	19.33
2311	CE1	PHE	A	111	-58.065	30.698	7.987	1.00	19.89
2312	CE2	PHE	A	111	-57.549	32.889	8.835	1.00	19.06
2313	CZ	PHE	A	111	-57.133	31.619	8.451	1.00	19.05
2314	N	THR	A	112	-60.72	31.295	5.228	1.00	19.67
2315	CA	THR	A	112	-60.611	30.081	4.445	1.00	17.65
2316	C	THR	A	112	-59.361	29.272	4.763	1.00	16.42
2317	O	THR	A	112	-58.265	29.816	4.85	1.00	16.46
2318	CB	THR	A	112	-60.614	30.438	2.943	1.00	18.46
2319	OG1	THR	A	112	-61.765	31.249	2.658	1.00	19.65

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## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

2320	CG2	THR	A	112	-60.656	29.165	2.077	1.00	17.83
2321	N	TYR	A	113	-59.539	27.967	4.94	1.00	16
2322	CA	TYR	A	113	-58.429	27.059	5.217	1.00	16.6
2323	C	TYR	A	113	-57.869	26.546	3.891	1.00	18.49
2324	O	TYR	A	113	-58.624	26.079	3.027	1.00	17.82
2325	CB	TYR	A	113	-58.903	25.852	6.031	1.00	15.92
2326	CG	TYR	A	113	-58.935	26.04	7.527	1.00	15.82
2327	CD1	TYR	A	113	-59.729	25.216	8.327	1.00	16.79
2328	CD2	TYR	A	113	-58.159	27.019	8.152	1.00	15.69
2329	CE1	TYR	A	113	-59.756	25.358	9.714	1.00	16.76
2330	CE2	TYR	A	113	-58.175	27.172	9.541	1.00	15.44
2331	CZ	TYR	A	113	-58.977	26.338	10.313	1.00	17.24
2332	OH	TYR	A	113	-59.009	26.478	11.678	1.00	17.25
2333	N	ALA	A	114	-56.552	26.633	3.726	1.00	18.8
2334	CA	ALA	A	114	-55.918	26.135	2.513	1.00	18.23
2335	C	ALA	A	114	-56.194	24.634	2.459	1.00	19.26
2336	O	ALA	A	114	-56.263	23.968	3.503	1.00	16.57
2337	CB	ALA	A	114	-54.412	26.393	2.554	1.00	17.63
2338	N	GLY	A	115	-56.342	24.115	1.242	1.00	19.35
2339	CA	GLY	A	115	-56.623	22.707	1.044	1.00	20.27
2340	C	GLY	A	115	-55.509	21.731	1.382	1.00	24.38
2341	O	GLY	A	115	-54.307	22.036	1.291	1.00	22.18
2342	N	ILE	A	116	-55.931	20.538	1.784	1.00	26.87
2343	CA	ILE	A	116	-55.018	19.467	2.13	1.00	31.6
2344	C	ILE	A	116	-55.399	18.245	1.303	1.00	36.17
2345	O	ILE	A	116	-56.258	17.453	1.692	1.00	35.59
2346	CB	ILE	A	116	-55.097	19.14	3.635	1.00	30.04
2347	CG1	ILE	A	116	-54.587	20.336	4.441	1.00	27.98
2348	CG2	ILE	A	116	-54.276	17.891	3.949	1.00	29.61
2349	CD1	ILE	A	116	-54.772	20.194	5.926	1.00	26.72
2350	N	ASP	A	117	-54.764	18.12	0.142	1.00	43
2351	CA	ASP	A	117	-55.012	17.006	-0.77	1.00	49.47
2352	C	ASP	A	117	-54.068	15.861	-0.418	1.00	52.4
2353	O	ASP	A	117	-52.036	15.87	-0.809	1.00	52.49
2354	CB	ASP	A	117	-54.781	17.458	-2.22	1.00	51.54
2355	CG	ASP	A	117	-54.856	16.309	-3.222	1.00	53.28
2356	OD1	ASP	A	117	-55.932	15.678	-3.345	1.00	54.18
2357	OD2	ASP	A	117	-53.833	16.045	-3.891	1.00	53.54
2358	N	CYS	A	118	-54.58	14.885	0.33	1.00	55.37
2359	CA	CYS	A	118	-53.781	13.733	0.743	1.00	58.82

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

2360	C	CYS	A	118	-53.504	12.775	-0.424	1.00	59.92
2361	O	CYS	A	118	-52.828	11.756	-0.254	1.00	60.11
2362	CB	CYS	A	118	-54.483	12.982	1.886	1.00	60.32
2363	SG	CYS	A	118	-54.65	13.918	3.448	1.00	62.94
2364	N	ALA	A	119	-54.027	13.111	-1.603	1.00	60.52
2365	CA	ALA	A	119	-53.828	12.296	-2.801	1.00	61.23
2366	C	ALA	A	119	-52.414	12.539	-3.321	1.00	61.74
2367	O	ALA	A	119	-51.881	11.76	-4.117	1.00	61.4
2368	CB	ALA	A	119	-54.861	12.666	-3.874	1.00	60.58
2369	N	ALA	A	120	-51.818	13.633	-2.855	1.00	62.06
2370	CA	ALA	A	120	-50.463	14.01	-3.233	1.00	62.53
2371	C	ALA	A	120	-49.543	13.833	-2.026	1.00	63.35
2372	O	ALA	A	120	-48.474	14.44	-1.956	1.00	64.1
2373	CB	ALA	A	120	-50.437	15.458	-3.702	1.00	61.63
2374	N	GLU	A	121	-49.971	12.999	-1.08	1.00	63.87
2375	CA	GLU	A	121	-49.203	12.733	0.135	1.00	64.12
2376	C	GLU	A	121	-49.176	11.243	0.478	1.00	64.54
2377	O	GLU	A	121	-49.817	10.858	1.478	1.00	65.25
2378	CB	GLU	A	121	-49.787	13.521	1.313	1.00	63.1
2379	CG	GLU	A	121	-49.62	15.031	1.196	1.00	62.45
2380	CD	GLU	A	121	-50.154	15.778	2.405	1.00	61.51
2381	OE1	GLU	A	121	-49.773	15.42	3.54	1.00	61.98
2382	OE2	GLU	A	121	-50.946	16.725	2.22	1.00	60.27
2383	OXT	GLU	A	121	-48.52	10.477	-0.262	1.00	65.04
2384	N	PRO	B	813	-59.975	-7.685	12.054	1.00	58.48
2385	CA	PRO	B	813	-60.084	-8.743	13.084	1.00	58.33
2386	C	PRO	B	813	-59.167	-8.44	14.261	1.00	58.25
2387	O	PRO	B	813	-58.255	-7.623	14.148	1.00	57.93
2388	CB	PRO	B	813	-59.683	-10.049	12.416	1.00	58.02
2389	CG	PRO	B	813	-58.715	-9.549	11.358	1.00	57.87
2390	CD	PRO	B	813	-59.353	-8.242	10.839	1.00	58.25
2391	N	THR	B	814	-59.407	-9.108	15.385	1.00	58.28
2392	CA	THR	B	814	-58.601	-8.907	16.585	1.00	57.39
2393	C	THR	B	814	-57.912	-10.184	17.064	1.00	57
2394	O	THR	B	814	-58.5	-11.265	17.056	1.00	56.65
2395	CB	THR	B	814	-59.463	-8.332	17.742	1.00	57.31
2396	OG1	THR	B	814	-58.784	-8.517	18.991	1.00	56.67
2397	CG2	THR	B	814	-60.822	-9.013	17.79	1.00	57.88
2398	N	ILE	B	815	-56.654	-10.047	17.472	1.00	57.06
2399	CA	ILE	B	815	-55.875	-11.174	17.974	1.00	56.43

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

2400	C	ILE	B	815	-55.704	-11.075	19.492	1.00	55.51
2401	O	ILE	B	815	-55.227	-10.066	20.016	1.00	55.48
2402	CB	ILE	B	815	-54.48	-11.24	17.302	1.00	56.8
2403	CG1	ILE	B	815	-53.54	-12.111	18.141	1.00	56.82
2404	CG2	ILE	B	815	-53.925	-9.845	17.11	1.00	57.68
2405	CD1	ILE	B	815	-52.151	-12.255	17.564	1.00	58.81
2406	N	TYR	B	816	-56.101	-12.133	20.191	1.00	53.8
2407	CA	TYR	B	816	-56.007	-12.168	21.643	1.00	52.6
2408	C	TYR	B	816	-54.799	-12.988	22.093	1.00	49.96
2409	O	TYR	B	816	-54.221	-13.742	21.311	1.00	50.31
2410	CB	TYR	B	816	-57.284	-12.77	22.245	1.00	54.71
2411	CG	TYR	B	816	-58.562	-12.216	21.66	1.00	57.19
2412	CD1	TYR	B	816	-59.102	-12.749	20.488	1.00	58.6
2413	CD2	TYR	B	816	-59.216	-11.138	22.258	1.00	57.95
2414	CE1	TYR	B	816	-60.261	-12.221	19.924	1.00	60.09
2415	CE2	TYR	B	816	-60.376	-10.601	21.701	1.00	59.08
2416	CZ	TYR	B	816	-60.892	-11.148	20.536	1.00	60.33
2417	OH	TYR	B	816	-62.036	-10.621	19.979	1.00	61.96
2418	N	PRO	B	817	-54.397	-12.839	23.363	1.00	47.13
2419	CA	PRO	B	817	-55.049	-11.941	24.322	1.00	45.23
2420	C	PRO	B	817	-54.763	-10.462	24.041	1.00	44.02
2421	O	PRC	B	817	-53.89	-10.125	23.239	1.00	43.37
2422	CB	PRO	B	817	-54.481	-12.405	25.661	1.00	45.44
2423	CG	PRO	B	817	-53.099	-12.871	25.292	1.00	45.19
2424	CD	PRO	B	817	-53.35	-13.643	24.02	1.00	46.01
2425	N	VAL	B	818	-55.518	-9.583	24.69	1.00	42.62
2426	CA	VAL	B	818	-55.32	-8.15	24.527	1.00	40.48
2427	C	VAL	B	818	-54.243	-7.732	25.518	1.00	39.55
2428	O	VAL	B	818	-54.342	-8.012	26.712	1.00	40.06
2429	CB	VAL	B	818	-56.622	-7.36	24.808	1.00	40.38
2430	CG1	VAL	B	818	-56.324	-5.869	24.901	1.00	40.46
2431	CG2	VAL	B	818	-57.629	-7.617	23.696	1.00	39.49
2432	N	LEU	B	819	-53.204	-7.08	25.014	1.00	38.09
2433	CA	LEU	B	819	-52.106	-6.64	25.858	1.00	37.27
2434	C	LEU	B	819	-52.219	-5.153	26.181	1.00	36.86
2435	O	LEU	B	819	-52.687	-4.359	25.363	1.00	35.32
2436	CB	LEU	B	819	-50.774	-6.917	25.157	1.00	38
2437	CG	LEU	B	819	-50.416	-8.379	24.868	1.00	37.8
2438	CD1	LEU	B	819	-49.229	-8.445	23.93	1.00	37.39
2439	CD2	LEU	B	819	-50.106	-9.096	26.175	1.00	37.76



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## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

2440	N	ASP	B	820	-51.8	-4.782	27.386	1.00	36.91
2441	CA	ASP	B	820	-51.835	-3.388	27.799	1.00	37.02
2442	C	ASP	B	820	-50.479	-2.741	27.556	1.00	35.19
2443	O	ASP	B	820	-49.458	-3.201	28.065	1.00	34.65
2444	CB	ASP	B	820	-52.203	-3.263	29.276	1.00	39.69
2445	CG	ASP	B	820	-51.975	-1.859	29.807	1.00	42.96
2446	OD1	ASP	B	820	-52.462	-0.893	29.177	1.00	45.79
2447	OD2	ASP	B	820	-51.306	-1.718	30.852	1.00	44.7
2448	N	TRP	B	821	-50.486	-1.671	26.772	1.00	33.83
2449	CA	TRP	B	821	-49.275	-0.941	26.431	1.00	32.73
2450	C	TRP	B	821	-48.33	-0.673	27.596	1.00	32.33
2451	O	TRP	B	821	-47.113	-0.681	27.426	1.00	32.95
2452	CB	TRP	B	821	-49.642	0.39	25.77	1.00	32.59
2453	CG	TRP	B	821	-48.466	1.29	25.587	1.00	31.35
2454	CD1	TRP	B	821	-48.043	2.277	26.434	1.00	30.51
2455	CD2	TRP	B	821	-47.506	1.229	24.529	1.00	30.5
2456	NE1	TRP	B	821	-46.875	2.832	25.97	1.00	30.02
2457	CE2	TRP	B	821	-46.521	2.207	24.802	1.00	30.27
2458	CE3	TRP	B	821	-47.38	0.441	23.377	1.00	30.29
2459	CZ2	TRP	B	821	-45.423	2.417	23.964	1.00	29.03
2460	CZ3	TRP	B	821	-46.288	0.651	22.542	1.00	30.28
2461	CH2	TRP	B	821	-45.323	1.634	22.842	1.00	30.28
2462	N	ASN	B	822	-48.882	-0.435	28.777	1.00	32.69
2463	CA	ASN	B	822	-48.054	-0.139	29.937	1.00	33.15
2464	C	ASN	B	822	-47.249	-1.303	30.492	1.00	32.94
2465	O	ASN	B	822	-46.275	-1.088	31.206	1.00	33.07
2466	CB	ASN	B	822	-48.907	0.476	31.04	1.00	34.44
2467	CG	ASN	B	822	-49.447	1.834	30.654	1.00	35.09
2468	OD1	ASN	B	822	-48.685	2.741	30.315	1.00	36.53
2469	ND2	ASN	B	822	-50.767	1.983	30.699	1.00	35.1
2470	N	ASP	B	823	-47.645	-2.532	30.175	1.00	33.31
2471	CA	ASP	B	823	-46.905	-3.693	30.656	1.00	33.27
2472	C	ASP	B	823	-45.755	-4.037	29.711	1.00	32.84
2473	O	ASP	B	823	-44.95	-4.922	30.005	1.00	34.57
2474	CB	ASP	B	823	-47.82	-4.914	30.786	1.00	35.49
2475	CG	ASP	B	823	-48.898	-4.739	31.844	1.00	37.25
2476	OD1	ASP	B	823	-48.567	-4.362	32.994	1.00	37.51
2477	OD2	ASP	B	823	-50.08	-4.994	31.522	1.00	37.22
2478	N	ILE	B	824	-45.678	-3.343	28.578	1.00	30.73
2479	CA	ILE	B	824	-44.631	-3.606	27.598	1.00	28.69

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

2480	C	ILE	B	824	-43.359	-2.813	27.853	1.00	29.19
2481	O	ILE	B	824	-43.377	-1.587	27.934	1.00	30.94
2482	CB	ILE	B	824	-45.114	-3.297	26.166	1.00	27.46
2483	CG1	ILE	B	824	-46.352	-4.136	25.849	1.00	25.51
2484	CG2	ILE	B	824	-43.997	-3.589	25.16	1.00	24.92
2485	CD1	ILE	B	824	-46.902	-3.903	24.461	1.00	24.56
2486	N	LYS	B	825	-42.249	-3.528	27.967	1.00	30.42
2487	CA	LYS	B	825	-40.957	-2.904	28.196	1.00	30.29
2488	C	LYS	B	825	-40.012	-3.295	27.065	1.00	28.41
2489	O	LYS	B	825	-39.613	-4.449	26.951	1.00	28.57
2490	CB	LYS	B	825	-40.384	-3.348	29.548	1.00	33.26
2491	CG	LYS	B	825	-39.095	-2.62	29.939	1.00	39.47
2492	CD	LYS	B	825	-38.75	-2.822	31.414	1.00	43.6
2493	CE	LYS	B	825	-37.44	-2.13	31.78	1.00	44.68
2494	NZ	LYS	B	825	-37.139	-2.236	33.236	1.00	45.86
2495	N	PHE	B	826	-39.676	-2.325	26.221	1.00	26.68
2496	CA	PHE	B	826	-38.781	-2.555	25.097	1.00	24.64
2497	C	PHE	B	826	-37.328	-2.592	25.557	1.00	24.03
2498	O	PHE	B	826	-36.874	-1.715	26.283	1.00	22.33
2499	CB	PHE	B	826	-38.966	-1.459	24.055	1.00	24.11
2500	CG	PHE	B	826	-40.38	-1.308	23.589	1.00	25.26
2501	CD1	PHE	B	826	-41.195	-0.312	24.111	1.00	26.71
2502	CD2	PHE	B	826	-40.906	-2.175	22.638	1.00	25.71
2503	CE1	PHE	B	826	-42.519	-0.18	23.692	1.00	27.37
2504	CE2	PHE	B	826	-42.224	-2.055	22.213	1.00	26.85
2505	CZ	PHE	B	826	-43.033	-1.056	22.741	1.00	27.7
2506	N	GLN	B	827	-36.595	-3.606	25.113	1.00	25.12
2507	CA	GLN	B	827	-35.206	-3.758	25.516	1.00	26.19
2508	C	GLN	B	827	-34.192	-3.624	24.39	1.00	26.16
2509	O	GLN	B	827	-33.076	-3.149	24.615	1.00	26.98
2510	CB	GLN	B	827	-35.016	-5.116	26.191	1.00	27.53
2511	CG	GLN	B	827	-36.065	-5.439	27.234	1.00	29.38
2512	CD	GLN	B	827	-36.027	-6.896	27.644	1.00	33.82
2513	OE1	GLN	B	827	-35.195	-7.314	28.453	1.00	36.01
2514	NE2	GLN	B	827	-36.922	-7.688	27.067	1.00	36.98
2515	N	ASP	B	828	-34.565	-4.035	23.182	1.00	25.6
2516	CA	ASP	B	828	-33.625	-3.969	22.068	1.00	25.39
2517	C	ASP	B	828	-34.334	-4.084	20.719	1.00	26
2518	O	ASP	B	828	-35.546	-4.313	20.646	1.00	26.38
2519	CB	ASP	B	828	-32.602	-5.111	22.204	1.00	25.47

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

2520	CG	ASP	B	828	-31.295	-4.844	21.455	1.00	26.42
2521	OD1	ASP	B	828	-31.284	-4.042	20.498	1.00	26.27
2522	OD2	ASP	B	828	-30.27	-5.458	21.821	1.00	25.71
2523	N	VAL	B	829	-33.558	-3.928	19.652	1.00	25.82
2524	CA	VAL	B	829	-34.056	-4.032	18.287	1.00	25.23
2525	C	VAL	B	829	-33.359	-5.251	17.686	1.00	25.03
2526	O	VAL	B	829	-32.134	-5.362	17.764	1.00	24.53
2527	CB	VAL	B	829	-33.674	-2.783	17.467	1.00	25.7
2528	CG1	VAL	B	829	-34.248	-2.877	16.07	1.00	25.2
2529	CG2	VAL	B	829	-34.171	-1.536	18.165	1.00	24.94
2530	N	ILE	B	830	-34.131	-6.168	17.109	1.00	23.99
2531	CA	ILE	B	830	-33.56	-7.378	16.508	1.00	23.88
2532	C	ILE	B	830	-34.348	-7.836	15.291	1.00	23.79
2533	O	ILE	B	830	-35.45	-7.354	15.026	1.00	24.51
2534	CB	ILE	B	830	-33.558	-8.582	17.484	1.00	23.14
2535	CG1	ILE	B	830	-35.002	-8.97	17.826	1.00	23.32
2536	CG2	ILE	B	830	-32.763	-8.252	18.735	1.00	24.38
2537	CD1	ILE	B	830	-35.143	-10.325	18.532	1.00	22.98
2538	N	GLY	B	831	-33.778	-8.786	14.56	1.00	22.57
2539	CA	GLY	B	831	-34.461	-9.324	13.401	1.00	21.5
2540	C	GLY	B	831	-35.053	-10.671	13.774	1.00	20.9
2541	O	GLY	B	831	-34.53	-11.365	14.65	1.00	20.68
2542	N	GLU	B	832	-36.152	-11.045	13.135	1.00	20.31
2543	CA	GLU	B	832	-36.765	-12.335	13.419	1.00	19.16
2544	C	GLU	B	832	-37.408	-12.935	12.182	1.00	18.1
2545	O	GLU	B	832	-38.616	-12.842	12.003	1.00	18.21
2546	CB	GLU	B	832	-37.811	-12.22	14.531	1.00	17.45
2547	CG	GLU	B	832	-38.314	-13.582	14.992	1.00	18.92
2548	CD	GLU	B	832	-38.927	-13.545	16.376	1.00	20.95
2549	OE1	GLU	B	832	-38.517	-12.681	17.172	1.00	20.11
2550	OE2	GLU	B	832	-39.8	-14.388	16.678	1.00	22.38
2551	N	GLY	B	833	-36.588	-13.556	11.337	1.00	17.15
2552	CA	GLY	B	833	-37.088	-14.175	10.121	1.00	16.77
2553	C	GLY	B	833	-37.669	-13.223	9.239	1.00	16.52
2554	O	GLY	B	833	-37.549	-12.034	9.162	1.00	17.61
2555	N	ASN	B	834	-38.905	-13.739	8.585	1.00	15.34
2556	CA	ASN	B	834	-39.723	-12.923	7.699	1.00	16.14
2557	C	ASN	B	834	-40.529	-11.844	8.425	1.00	16.45
2558	O	ASN	B	834	-41.314	-11.135	7.796	1.00	16.67
2559	CB	ASN	B	834	-40.649	-13.81	6.852	1.00	14.8

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

2560	CG	ASN	B	834	-41.487	-14.765	7.691	1.00	16.42
2561	OD1	ASN	B	834	-42.014	-15.755	7.174	1.00	18.97
2562	ND2	ASN	B	834	-41.619	-14.475	8.981	1.00	10.95
2563	N	PHE	B	835	-40.344	-11.731	9.743	1.00	15.16
2564	CA	PHE	B	835	-41.028	-10.698	10.524	1.00	15.68
2565	C	PHE	B	835	-40.238	-9.411	10.337	1.00	17.31
2566	O	PHE	B	835	-40.756	-8.316	10.534	1.00	17.37
2567	CB	PHE	B	835	-41.05	-11.025	12.031	1.00	16.85
2568	CG	PHE	B	835	-42.186	-11.921	12.461	1.00	17.04
2569	CD1	PHE	B	835	-42.033	-13.309	12.484	1.00	15.53
2570	CD2	PHE	B	835	-43.416	-11.372	12.836	1.00	16.82
2571	CE1	PHE	B	835	-43.091	-14.138	12.873	1.00	15.92
2572	CE2	PHE	B	835	-44.481	-12.192	13.225	1.00	16.4
2573	CZ	PHE	B	835	-44.316	-13.578	13.244	1.00	17.25
2574	N	GLY	B	836	-38.971	-9.556	9.959	1.00	18.23
2575	CA	GLY	B	836	-38.12	-8.401	9.76	1.00	18.64
2576	C	GLY	B	836	-37.588	-7.92	11.094	1.00	21.7
2577	O	GLY	B	836	-37.321	-8.726	11.994	1.00	20.22
2578	N	GLN	B	837	-37.431	-6.608	11.227	1.00	23.1
2579	CA	GLN	B	837	-36.943	-6.029	12.469	1.00	24.6
2580	C	GLN	B	837	-38.088	-5.998	13.477	1.00	23.18
2581	O	GLN	B	837	-39.196	-5.568	13.156	1.00	22.4
2582	CB	GLN	B	837	-36.43	-4.608	12.23	1.00	28.3
2583	CG	GLN	B	837	-35.387	-4.501	11.126	1.00	35.91
2584	CD	GLN	B	837	-34.206	-5.433	11.346	1.00	40.25
2585	OE1	GLN	B	837	-33.547	-5.384	12.386	1.00	42.95
2586	NE2	GLN	B	837	-33.933	-6.289	10.363	1.00	40.84
2587	N	VAL	B	838	-37.815	-6.47	14.69	1.00	20.49
2588	CA	VAL	B	838	-38.807	-6.487	15.755	1.00	19.3
2589	C	VAL	B	838	-38.124	-5.982	17.017	1.00	19.46
2590	O	VAL	B	838	-36.899	-5.911	17.077	1.00	18.77
2591	CB	VAL	B	838	-39.374	-7.92	16.006	1.00	18.27
2592	CG1	VAL	B	838	-40.046	-8.44	14.75	1.00	18.14
2593	CG2	VAL	B	838	-38.27	-8.869	16.43	1.00	17.48
2594	N	LEU	B	839	-38.914	-5.626	18.021	1.00	20.59
2595	CA	LEU	B	839	-38.362	-5.118	19.274	1.00	20.55
2596	C	LEU	B	839	-38.32	-6.197	20.343	1.00	20.19
2597	O	LEU	B	839	-39.349	-6.765	20.691	1.00	18.64
2598	CB	LEU	B	839	-39.217	-3.96	19.787	1.00	19.95
2599	CG	LEU	B	839	-39.387	-2.764	18.848	1.00	21.08

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

2600	CD1	LEU	B	839	-40.631	-2.002	19.226	1.00	21.72
2601	CD2	LEU	B	839	-38.159	-1.873	18.914	1.00	20.71
2602	N	LYS	B	840	-37.136	-6.493	20.861	1.00	21.41
2603	CA	LYS	B	840	-37.047	-7.48	21.929	1.00	24.14
2604	C	LYS	B	840	-37.657	-6.795	23.149	1.00	23.82
2605	O	LYS	B	840	-37.295	-5.666	23.487	1.00	23.05
2606	CB	LYS	B	840	-35.589	-7.861	22.219	1.00	26.33
2607	CG	LYS	B	840	-35.43	-8.94	23.296	1.00	28.72
2608	CD	LYS	B	840	-33.968	-9.339	23.471	1.00	30.67
2609	CE	LYS	B	840	-33.807	-10.436	24.517	1.00	31.96
2610	NZ	LYS	B	840	-34.193	-10.003	25.893	1.00	34.43
2611	N	ALA	B	841	-38.592	-7.465	23.804	1.00	23.88
2612	CA	ALA	B	841	-39.225	-6.866	24.961	1.00	25.91
2613	C	ALA	B	841	-39.647	-7.882	26.009	1.00	26.91
2614	O	ALA	B	841	-39.355	-9.074	25.91	1.00	27.33
2615	CB	ALA	B	841	-40.436	-6.059	24.513	1.00	25.5
2616	N	ARG	B	842	-40.31	-7.371	27.037	1.00	28.75
2617	CA	ARG	B	842	-40.857	-8.184	28.107	1.00	29.7
2618	C	ARG	B	842	-42.296	-7.712	28.193	1.00	29.77
2619	O	ARG	B	842	-42.559	-6.515	28.283	1.00	29.29
2620	CB	ARG	B	842	-40.139	-7.937	29.439	1.00	30.34
2621	CG	ARG	B	842	-38.672	-8.327	29.425	1.00	33.71
2622	CD	ARG	B	842	-38.238	-8.933	30.747	1.00	38.41
2623	NE	ARG	B	842	-38.909	-10.205	31.013	1.00	43.07
2624	CZ	ARG	B	842	-38.682	-10.967	32.08	1.00	44.73
2625	NH1	ARG	B	842	-37.796	-10.59	32.993	1.00	45.43
2626	NH2	ARG	B	842	-39.339	-12.11	32.235	1.00	46.75
2627	N	ILE	B	843	-43.228	-8.651	28.113	1.00	31.3
2628	CA	ILE	B	843	-44.639	-8.319	28.193	1.00	31.74
2629	C	ILE	B	843	-45.216	-9.04	29.403	1.00	33.28
2630	O	ILE	B	843	-44.547	-9.878	30.007	1.00	31.81
2631	CB	ILE	B	843	-45.39	-8.772	26.927	1.00	29.87
2632	CG1	ILE	B	843	-45.435	-10.301	26.861	1.00	29.37
2633	CG2	ILE	B	843	-44.69	-8.222	25.695	1.00	28.78
2634	CD1	ILE	B	843	-46.408	-10.847	25.837	1.00	27.25
2635	N	LYS	B	844	-46.448	-8.702	29.764	1.00	36.34
2636	CA	LYS	B	844	-47.099	-9.344	30.894	1.00	40.52
2637	C	LYS	B	844	-48.28	-10.145	30.368	1.00	41.55
2638	O	LYS	B	844	-49.223	-9.585	29.81	1.00	42.4
2639	CB	LYS	B	844	-47.583	-8.304	31.909	1.00	43.2

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TABLE 3

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

2640	CG	LYS	B	844	-48.207	-8.91	33.17	1.00	46.51
2641	CD	LYS	B	844	-48.657	-7.833	34.164	1.00	48.29
2642	CE	LYS	B	844	-49.166	-8.455	35.468	1.00	49.72
2643	NZ	LYS	B	844	-49.48	-7.444	36.533	1.00	48.73
2644	N	LYS	B	845	-48.209	-11.462	30.527	1.00	42.27
2645	CA	LYS	B	845	-49.272	-12.351	30.08	1.00	43.27
2646	C	LYS	B	845	-49.555	-13.352	31.195	1.00	44.17
2647	O	LYS	B	845	-48.627	-13.848	31.848	1.00	43.07
2648	CB	LYS	B	845	-48.855	-13.08	28.802	1.00	43.19
2649	CG	LYS	B	845	-49.914	-14.015	28.261	1.00	43.86
2650	CD	LYS	B	845	-49.531	-14.559	26.895	1.00	44.34
2651	CE	LYS	B	845	-50.636	-15.442	26.343	1.00	44.53
2652	NZ	LYS	B	845	-50.308	-15.954	24.99	1.00	45.92
2653	N	ASP	B	846	-50.835	-13.64	31.414	1.00	44.78
2654	CA	ASP	B	846	-51.241	-14.565	32.469	1.00	46.07
2655	C	ASP	B	846	-50.662	-14.115	33.808	1.00	45.73
2656	O	ASP	B	846	-50.473	-14.928	34.714	1.00	45.93
2657	CB	ASP	B	846	-50.759	-15.99	32.167	1.00	48.32
2658	CG	ASP	B	846	-51.366	-16.557	30.9	1.00	50.28
2659	OD1	ASP	B	846	-52.607	-16.499	30.76	1.00	50.49
2660	OD2	ASP	B	846	-50.602	-17.068	30.049	1.00	51.46
2661	N	GLY	B	847	-50.373	-12.821	33.924	1.00	44.97
2662	CA	GLY	B	847	-49.817	-12.299	35.161	1.00	44.16
2663	C	GLY	B	847	-48.314	-12.476	35.26	1.00	44.27
2664	O	GLY	B	847	-47.683	-11.981	36.194	1.00	44.22
2665	N	LEU	B	848	-47.735	-13.179	34.293	1.00	44.14
2666	CA	LEU	B	848	-46.296	-13.415	34.281	1.00	44.55
2667	C	LEU	B	848	-45.525	-12.416	33.425	1.00	44.51
2668	O	LEU	B	848	-46.076	-11.782	32.526	1.00	44.96
2669	CB	LEU	B	848	-45.993	-14.816	33.756	1.00	44.56
2670	CG	LEU	B	848	-46.338	-16.027	34.611	1.00	45.26
2671	CD1	LEU	B	848	-46.034	-17.291	33.818	1.00	44.69
2672	CD2	LEU	B	848	-45.533	-15.994	35.898	1.00	45.87
2673	N	ARG	B	849	-44.237	-12.29	33.722	1.00	44.86
2674	CA	ARG	B	849	-43.344	-11.42	32.971	1.00	44.44
2675	C	ARG	B	849	-42.546	-12.346	32.056	1.00	42.58
2676	O	ARG	B	849	-41.777	-13.187	32.529	1.00	42.41
2677	CB	ARG	B	849	-42.397	-10.674	33.915	1.00	47.54
2678	CG	ARG	B	849	-43.031	-9.485	34.616	1.00	53.03
2679	CD	ARG	B	849	-43.339	-8.386	33.617	1.00	56.95

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

2680	NE	ARG	B	849	-44.095	-7.289	34.212	1.00	60.88
2681	CZ	ARG	B	849	-44.464	-6.199	33.547	1.00	62.01
2682	NH1	ARG	B	849	-45.153	-5.244	34.159	1.00	62.51
2683	NH2	ARG	B	849	-44.139	-6.068	32.267	1.00	62.03
2684	N	MET	B	850	-42.732	-12.204	30.75	1.00	38.92
2685	CA	MET	B	850	-42.028	-13.063	29.816	1.00	36.12
2686	C	MET	B	850	-41.364	-12.319	28.667	1.00	33.8
2687	O	MET	B	850	-41.822	-11.261	28.246	1.00	32.91
2688	CB	MET	B	850	-42.99	-14.103	29.239	1.00	36.3
2689	CG	MET	B	850	-44.084	-13.509	28.37	1.00	36.06
2690	SD	MET	B	850	-44.855	-14.744	27.335	1.00	36.48
2691	CE	MET	B	850	-46.289	-15.171	28.311	1.00	39.91
2692	N	ASP	B	851	-40.278	-12.899	28.166	1.00	32.2
2693	CA	ASP	B	851	-39.541	-12.347	27.039	1.00	29.16
2694	C	ASP	B	851	-40.395	-12.526	25.796	1.00	26.58
2695	O	ASP	B	851	-41.186	-13.466	25.698	1.00	25.67
2696	CB	ASP	B	851	-38.222	-13.093	26.833	1.00	31.13
2697	CG	ASP	B	851	-37.23	-12.852	27.949	1.00	33.49
2698	OD1	ASP	B	851	-36.148	-13.469	27.904	1.00	35.27
2699	OD2	ASP	B	851	-37.527	-12.053	28.866	1.00	34.82
2700	N	ALA	B	852	-40.231	-11.622	24.844	1.00	24.03
2701	CA	ALA	B	852	-40.989	-11.693	23.612	1.00	22.09
2702	C	ALA	B	852	-40.401	-10.712	22.63	1.00	20.5
2703	O	ALA	B	852	-39.444	-10.002	22.94	1.00	20
2704	CB	ALA	B	852	-42.444	-11.355	23.876	1.00	22.15
2705	N	ALA	B	853	-40.97	-10.693	21.434	1.00	19.53
2706	CA	ALA	B	853	-40.533	-9.78	20.39	1.00	20.42
2707	C	ALA	B	853	-41.792	-9.06	19.922	1.00	20.7
2708	O	ALA	B	853	-42.883	-9.642	19.935	1.00	21.17
2709	CB	ALA	B	853	-39.901	-10.552	19.24	1.00	18.79
2710	N	ILE	B	854	-41.653	-7.803	19.515	1.00	20.63
2711	CA	ILE	B	854	-42.813	-7.048	19.067	1.00	20.68
2712	C	ILE	B	854	-42.673	-6.486	17.662	1.00	21.29
2713	O	ILE	B	854	-41.751	-5.735	17.356	1.00	20.67
2714	CB	ILE	B	854	-43.148	-5.915	20.061	1.00	21.24
2715	CG1	ILE	B	854	-43.665	-6.534	21.363	1.00	23.18
2716	CG2	ILE	B	854	-44.181	-4.966	19.469	1.00	18.56
2717	CD1	ILE	B	854	-44.089	-5.532	22.4	1.00	26.8
2718	N	LYS	B	855	-43.609	-6.89	16.815	1.00	21.67
2719	CA	LYS	B	855	-43.677	-6.469	15.434	1.00	21.75

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TABLE 3

STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

2720	C	LYS	B	855	-44.697	-5.35	15.375	1.00	23.07
2721	O	LYS	B	855	-45.87	-5.575	15.65	1.00	23.06
2722	CB	LYS	B	855	-44.151	-7.638	14.559	1.00	21.89
2723	CG	LYS	B	855	-44.425	-7.281	13.095	1.00	19.24
2724	CD	LYS	B	855	-43.174	-6.792	12.402	1.00	18.32
2725	CE	LYS	B	855	-43.419	-6.574	10.913	1.00	19.4
2726	NZ	LYS	B	855	-42.205	-6.069	10.212	1.00	14.81
2727	N	ARG	B	856	-44.25	-4.147	15.033	1.00	25.71
2728	CA	ARG	B	856	-45.156	-3.014	14.926	1.00	27.66
2729	C	ARG	B	856	-45.727	-2.988	13.507	1.00	28.97
2730	O	ARG	B	856	-44.985	-3.025	12.528	1.00	28.21
2731	CB	ARG	B	856	-44.419	-1.703	15.221	1.00	29.33
2732	CG	ARG	B	856	-45.362	-0.534	15.47	1.00	30.6
2733	CD	ARG	B	856	-44.635	0.741	15.839	1.00	32.05
2734	NE	ARG	B	856	-43.994	1.361	14.688	1.00	35.86
2735	CZ	ARG	B	856	-44.083	2.654	14.397	1.00	36.67
2736	NH1	ARG	B	856	-44.79	3.462	15.177	1.00	36.55
2737	NH2	ARG	B	856	-43.469	3.135	13.322	1.00	37.8
2738	N	MET	B	857	-47.049	-2.925	13.403	1.00	30.91
2739	CA	MET	B	857	-47.714	-2.915	12.106	1.00	34.45
2740	C	MET	B	857	-48.558	-1.66	11.927	1.00	36.55
2741	O	MET	B	857	-49.301	-1.271	12.833	1.00	36.61
2742	CB	MET	B	857	-48.603	-4.159	11.972	1.00	33.78
2743	CG	MET	B	857	-47.828	-5.473	11.962	1.00	35.17
2744	SD	MET	B	857	-48.832	-6.933	12.345	1.00	35.62
2745	CE	MET	B	857	-49.794	-7.115	10.805	1.00	35.34
2746	N	ALA	B	858	-48.437	-1.029	10.76	1.00	39.73
2747	CA	ALA	B	858	-49.204	0.181	10.455	1.00	43.33
2748	C	ALA	B	858	-50.615	-0.212	10.021	1.00	45.64
2749	O	ALA	B	858	-50.804	-0.815	8.963	1.00	44.16
2750	CB	ALA	B	858	-48.512	0.988	9.35	1.00	42.93
2751	N	GLU	B	859	-51.598	0.13	10.851	1.00	49.13
2752	CA	GLU	B	859	-52.991	-0.197	10.576	1.00	53.08
2753	C	GLU	B	859	-53.559	0.579	9.389	1.00	55.54
2754	O	GLU	B	859	-54.128	-0.013	8.47	1.00	55.73
2755	CB	GLU	B	859	-53.848	0.047	11.827	1.00	53.7
2756	CG	GLU	B	859	-53.452	-0.819	13.023	1.00	55.82
2757	CD	GLU	B	859	-54.432	-0.733	14.186	1.00	57.01
2758	OE1	GLU	B	859	-54.596	0.367	14.754	1.00	58.17
2759	OE2	GLU	B	859	-55.038	-1.772	14.534	1.00	57.4



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## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

2760	N	ALA	B	860	-53.405	1.899	9.406	1.00	57.92
2761	CA	ALA	B	860	-53.913	2.729	8.317	1.00	60.22
2762	CB	ALA	B	860	-54.249	4.13	8.835	1.00	60.72
2763	C	ALA	B	860	-52.888	2.815	7.187	1.00	61.22
2764	OT1	ALA	B	860	-52.592	3.946	6.739	1.00	61.47
2765	OT2	ALA	B	860	-52.399	1.745	6.758	1.00	62.08
2766	N	ALA	B	867	-57.828	-4.059	3.223	1.00	56.23
2767	CA	ALA	B	867	-56.52	-3.343	3.279	1.00	55.91
2768	C	ALA	B	867	-55.361	-4.332	3.269	1.00	55.4
2769	O	ALA	B	867	-55.549	-5.528	3.488	1.00	54.63
2770	CB	ALA	B	867	-56.45	-2.471	4.536	1.00	55.3
2771	N	ASP	B	868	-54.164	-3.816	3.011	1.00	55.53
2772	CA	ASP	B	868	-52.948	-4.624	2.976	1.00	55.59
2773	C	ASP	B	868	-52.705	-5.17	4.387	1.00	55.21
2774	O	ASP	B	868	-52.233	-6.295	4.57	1.00	54.41
2775	CB	ASP	B	868	-51.77	-3.744	2.545	1.00	56.71
2776	CG	ASP	B	868	-50.581	-4.546	2.065	1.00	58.16
2777	OD1	ASP	B	868	-50.096	-5.414	2.824	1.00	60.34
2778	OD2	ASP	B	868	-50.126	-4.3	0.926	1.00	58.32
2779	N	PHE	B	869	-53.049	-4.344	5.372	1.00	54.66
2780	CA	PHE	B	869	-52.904	-4.661	6.789	1.00	53.29
2781	C	PHE	B	869	-53.918	-5.709	7.254	1.00	52.13
2782	O	PHE	B	869	-53.549	-6.716	7.858	1.00	51.69
2783	CB	PHE	B	869	-53.073	-3.377	7.608	1.00	53.32
2784	CG	PHE	B	869	-53.091	-3.597	9.091	1.00	53.66
2785	CD1	PHE	B	869	-51.947	-4.015	9.761	1.00	53.98
2786	CD2	PHE	B	869	-54.258	-3.391	9.82	1.00	53.71
2787	CE1	PHE	B	869	-51.984	-4.225	11.141	1.00	54.09
2788	CE2	PHE	B	869	-54.286	-3.598	11.198	1.00	53.85
2789	CZ	PHE	B	869	-53.137	-4.016	11.86	1.00	53.59
2790	N	ALA	B	870	-55.195	-5.461	6.976	1.00	51.34
2791	CA	ALA	B	870	-56.261	-6.378	7.371	1.00	50.02
2792	C	ALA	B	870	-56.09	-7.741	6.711	1.00	48.73
2793	O	ALA	B	870	-56.629	-8.743	7.184	1.00	48.97
2794	CB	ALA	B	870	-57.619	-5.792	7.01	1.00	49.28
2795	N	GLY	B	871	-55.342	-7.77	5.613	1.00	47.01
2796	CA	GLY	B	871	-55.108	-9.022	4.919	1.00	44.91
2797	C	GLY	B	871	-54.151	-9.905	5.698	1.00	43.42
2798	O	GLY	B	871	-54.431	-11.075	5.944	1.00	42.15
2799	N	GLU	B	872	-53.02	-9.334	6.097	1.00	43.04

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## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

2800	CA	GLU	B	872	-52.011	-10.067	6.849	1.00	43.83
2801	C	GLU	B	872	-52.47	-10.423	8.257	1.00	42.48
2802	O	GLU	B	872	-51.943	-11.349	8.875	1.00	43.32
2803	CB	GLU	B	872	-50.72	-9.251	6.907	1.00	45.29
2804	CG	GLU	B	872	-50.143	-8.989	5.527	1.00	50.22
2805	CD	GLU	B	872	-48.783	-8.332	5.569	1.00	52.36
2806	OE1	GLU	B	872	-48.69	-7.176	6.041	1.00	53.14
2807	OE2	GLU	B	872	-47.807	-8.982	5.13	1.00	52.43
2808	N	LEU	B	873	-53.458	-9.688	8.757	1.00	40.42
2809	CA	LEU	B	873	-53.996	-9.925	10.088	1.00	38.57
2810	C	LEU	B	873	-54.96	-11.104	10.014	1.00	37.79
2811	O	LEU	B	873	-55.034	-11.928	10.927	1.00	36.29
2812	CB	LEU	B	873	-54.729	-8.674	10.575	1.00	39.73
2813	CG	LEU	B	873	-55.2	-8.608	12.028	1.00	40.04
2814	CD1	LEU	B	873	-54	-8.534	12.965	1.00	40.34
2815	CD2	LEU	B	873	-56.079	-7.377	12.206	1.00	41.89
2816	N	GLU	B	874	-55.694	-11.176	8.909	1.00	37.62
2817	CA	GLU	B	874	-56.653	-12.248	8.686	1.00	37.54
2818	C	GLU	B	874	-55.912	-13.578	8.658	1.00	35.58
2819	O	GLU	B	874	-56.433	-14.599	9.101	1.00	36.61
2820	CB	GLU	B	874	-57.387	-12.033	7.355	1.00	40.64
2821	CG	GLU	B	874	-58.524	-13.017	7.095	1.00	43.7
2822	CD	GLU	B	874	-59.151	-12.842	5.719	1.00	45.99
2823	OE1	GLU	B	874	-59.637	-11.73	5.415	1.00	48.09
2824	OE2	GLU	B	874	-59.161	-13.819	4.938	1.00	46.69
2825	N	VAL	B	875	-54.689	-13.558	8.139	1.00	33.26
2826	CA	VAL	B	875	-53.879	-14.767	8.061	1.00	31.32
2827	C	VAL	B	875	-53.225	-15.121	9.398	1.00	30.98
2828	O	VAL	B	875	-53.191	-16.289	9.778	1.00	30.28
2829	CB	VAL	B	875	-52.784	-14.63	6.985	1.00	30.59
2830	CG1	VAL	B	875	-51.902	-15.873	6.973	1.00	26.72
2831	CG2	VAL	B	875	-53.43	-14.417	5.617	1.00	27.5
2832	N	LEU	B	876	-52.71	-14.12	10.108	1.00	30.28
2833	CA	LEU	B	876	-52.087	-14.357	11.402	1.00	31.27
2834	C	LEU	B	876	-53.002	-15.028	12.416	1.00	32.44
2835	O	LEU	B	876	-52.567	-15.842	13.232	1.00	33.08
2836	CB	LEU	B	876	-51.543	-13.039	11.984	1.00	29.54
2837	CG	LEU	B	876	-50.35	-12.389	11.277	1.00	29.48
2838	CD1	LEU	B	876	-50.158	-10.977	11.791	1.00	28.76
2839	CD2	LEU	B	876	-49.091	-13.222	11.506	1.00	28.16

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

2840	N	CYS	B	877	-54.283	-14.686	12.362	1.00	33.12
2841	CA	CYS	B	877	-55.261	-15.255	13.28	1.00	35.33
2842	C	CYS	B	877	-55.524	-16.735	13.033	1.00	34.55
2843	O	CYS	B	877	-55.934	-17.458	13.94	1.00	35.5
2844	CB	CYS	B	877	-56.583	-14.488	13.182	1.00	38.79
2845	SG	CYS	B	877	-56.488	-12.782	13.772	1.00	46.2
2846	N	LYS	B	878	-55.289	-17.184	11.806	1.00	32.4
2847	CA	LYS	B	878	-55.516	-18.577	11.459	1.00	30.34
2848	C	LYS	B	878	-54.336	-19.48	11.808	1.00	27.62
2849	O	LYS	B	878	-54.424	-20.699	11.684	1.00	27.24
2850	CB	LYS	B	878	-55.828	-18.698	9.965	1.00	32.31
2851	CG	LYS	B	878	-57.008	-17.857	9.507	1.00	36.2
2852	CD	LYS	B	878	-58.272	-18.195	10.29	1.00	39.88
2853	CE	LYS	B	878	-59.443	-17.305	9.878	1.00	41.71
2854	NZ	LYS	B	878	-59.795	-17.476	8.435	1.00	42.59
2855	N	LEU	B	879	-53.235	-18.891	12.253	1.00	25.99
2856	CA	LEU	B	879	-52.059	-19.687	12.587	1.00	24.51
2857	C	LEU	B	879	-52.316	-20.695	13.699	1.00	24.71
2858	O	LEU	B	879	-51.887	-21.845	13.608	1.00	25.93
2859	CB	LEU	B	879	-50.895	-18.779	12.984	1.00	21.59
2860	CG	LEU	B	879	-50.151	-18.076	11.846	1.00	21.01
2861	CD1	LEU	B	879	-49.276	-16.975	12.425	1.00	20.05
2862	CD2	LEU	B	879	-49.314	-19.081	11.058	1.00	19.19
2863	N	GLY	B	880	-53.022	-20.271	14.741	1.00	23.53
2864	CA	GLY	B	880	-53.285	-21.169	15.848	1.00	22.86
2865	C	GLY	B	880	-52.009	-21.334	16.647	1.00	22.66
2866	O	GLY	B	880	-51.193	-20.418	16.704	1.00	22.73
2867	N	HIS	B	881	-51.812	-22.498	17.253	1.00	22.76
2868	CA	HIS	B	881	-50.605	-22.719	18.042	1.00	22.61
2869	C	HIS	B	881	-49.94	-24.059	17.802	1.00	20.88
2870	O	HIS	B	881	-50.601	-25.099	17.698	1.00	19.52
2871	CB	HIS	B	881	-50.904	-22.564	19.533	1.00	23.83
2872	CG	HIS	B	881	-51.252	-21.166	19.925	1.00	28.1
2873	ND1	HIS	B	881	-50.344	-20.131	19.864	1.00	31.79
2874	CD2	HIS	B	881	-52.415	-20.621	20.353	1.00	29.95
2875	CE1	HIS	B	881	-50.933	-19.009	20.237	1.00	32.71
2876	NE2	HIS	B	881	-52.191	-19.279	20.539	1.00	31.93
2877	N	HIS	B	882	-48.614	-24.011	17.728	1.00	17.28
2878	CA	HIS	B	882	-47.804	-25.195	17.509	1.00	14.7
2879	C	HIS	B	882	-46.396	-24.88	18.008	1.00	14.61

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

2880	O	HIS	B	882	-45.908	-23.757	17.87	1.00	13.48
2881	CB	HIS	B	882	-47.796	-25.563	16.02	1.00	12.34
2882	CG	HIS	B	882	-47.227	-26.918	15.743	1.00	11.51
2883	ND1	HIS	B	882	-45.874	-27.186	15.804	1.00	11.45
2884	CD2	HIS	B	882	-47.831	-28.094	15.455	1.00	8.44
2885	CE1	HIS	B	882	-45.672	-28.469	15.567	1.00	9.54
2886	NE2	HIS	B	882	-46.842	-29.042	15.352	1.00	10.59
2887	N	PRO	B	883	-45.726	-25.872	18.609	1.00	14.5
2888	CA	PRO	B	883	-44.369	-25.699	19.141	1.00	13.88
2889	C	PRO	B	883	-43.341	-25.359	18.069	1.00	14.34
2890	O	PRO	B	883	-42.318	-24.725	18.354	1.00	13.76
2891	CB	PRO	B	883	-44.067	-27.055	19.776	1.00	14.5
2892	CG	PRO	B	883	-45.423	-27.647	20.032	1.00	14.05
2893	CD	PRO	B	883	-46.204	-27.246	18.826	1.00	11.71
2894	N	ASN	B	884	-43.613	-25.78	16.837	1.00	12.06
2895	CA	ASN	B	884	-42.668	-25.553	15.759	1.00	11.88
2896	C	ASN	B	884	-42.917	-24.361	14.836	1.00	12.1
2897	O	ASN	B	884	-42.367	-24.292	13.734	1.00	12.98
2898	CB	ASN	B	884	-42.502	-26.853	14.969	1.00	10.8
2899	CG	ASN	B	884	-41.951	-27.976	15.835	1.00	10.51
2900	OD1	ASN	B	884	-42.543	-29.051	15.938	1.00	9.84
2901	ND2	ASN	B	884	-40.815	-27.72	16.476	1.00	8.18
2902	N	ILE	B	885	-43.755	-23.431	15.28	1.00	10.89
2903	CA	ILE	B	885	-43.987	-22.206	14.525	1.00	12.33
2904	C	ILE	B	885	-43.811	-21.112	15.557	1.00	13.36
2905	O	ILE	B	885	-43.816	-21.389	16.762	1.00	14.93
2906	CB	ILE	B	885	-45.423	-22.073	13.931	1.00	11.48
2907	CG1	ILE	B	885	-46.456	-21.98	15.058	1.00	12.38
2908	CG2	ILE	B	885	-45.704	-23.22	12.955	1.00	8.92
2909	CD1	ILE	B	885	-47.882	-21.716	14.569	1.00	10.21
2910	N	ILE	B	886	-43.61	-19.886	15.096	1.00	11.86
2911	CA	ILE	B	886	-43.485	-18.77	16.012	1.00	11.16
2912	C	ILE	B	886	-44.924	-18.484	16.423	1.00	11.4
2913	O	ILE	B	886	-45.772	-18.2	15.581	1.00	9.28
2914	CB	ILE	B	886	-42.873	-17.525	15.31	1.00	11.68
2915	CG1	ILE	B	886	-41.362	-17.718	15.139	1.00	9.36
2916	CG2	ILE	B	886	-43.2	-16.253	16.088	1.00	8.3
2917	CD1	ILE	B	886	-40.587	-17.772	16.431	1.00	9.18
2918	N	ASN	B	887	-45.199	-18.573	17.719	1.00	12.91
2919	CA	ASN	B	887	-46.543	-18.339	18.219	1.00	14.41

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## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

2920	C	ASN	B	887	-46.829	-16.89	18.597	1.00	15.28
2921	O	ASN	B	887	-45.96	-16.184	19.109	1.00	14.37
2922	CB	ASN	B	887	-46.807	-19.249	19.422	1.00	16.35
2923	CG	ASN	B	887	-46.867	-20.721	19.036	1.00	17.53
2924	OD1	ASN	B	887	-47.851	-21.18	18.453	1.00	17.64
2925	ND2	ASN	B	887	-45.802	-21.464	19.346	1.00	16.27
2926	N	LEU	B	888	-48.054	-16.451	18.321	1.00	16.41
2927	CA	LEU	B	888	-48.479	-15.101	18.66	1.00	17.76
2928	C	LEU	B	888	-48.86	-15.124	20.144	1.00	18.38
2929	O	LEU	B	888	-49.612	-15.99	20.588	1.00	18.45
2930	CB	LEU	B	888	-49.67	-14.69	17.791	1.00	17.88
2931	CG	LEU	B	888	-49.44	-14.834	16.279	1.00	18.87
2932	CD1	LEU	B	888	-50.641	-14.277	15.533	1.00	19.71
2933	CD2	LEU	B	888	-48.174	-14.106	15.855	1.00	16.31
2934	N	LEU	B	889	-48.323	-14.18	20.907	1.00	18.92
2935	CA	LEU	B	889	-48.573	-14.123	22.342	1.00	20.65
2936	C	LEU	B	889	-49.637	-13.099	22.751	1.00	22.78
2937	O	LEU	B	889	-50.124	-13.122	23.877	1.00	25.68
2938	CB	LEU	B	889	-47.258	-13.824	23.072	1.00	18.03
2939	CG	LEU	B	889	-46.086	-14.771	22.792	1.00	17.82
2940	CD1	LEU	B	889	-44.839	-14.291	23.531	1.00	15.21
2941	CD2	LEU	B	889	-46.456	-16.189	23.228	1.00	15.74
2942	N	GLY	B	890	-49.999	-12.213	21.832	1.00	24.97
2943	CA	GLY	B	890	-50.99	-11.193	22.122	1.00	25.65
2944	C	GLY	B	890	-50.749	-9.954	21.279	1.00	26.37
2945	O	GLY	B	890	-49.761	-9.876	20.55	1.00	25.82
2946	N	ALA	B	891	-51.642	-8.977	21.378	1.00	27.44
2947	CA	ALA	B	891	-51.503	-7.761	20.595	1.00	28.37
2948	C	ALA	B	891	-52.051	-6.55	21.328	1.00	30.21
2949	O	ALA	B	891	-52.88	-6.679	22.234	1.00	28.56
2950	CB	ALA	B	891	-52.211	-7.927	19.265	1.00	28.63
2951	N	CYS	B	892	-51.581	-5.372	20.919	1.00	32.21
2952	CA	CYS	B	892	-51.997	-4.11	21.524	1.00	33.74
2953	C	CYS	B	892	-52.078	-2.963	20.515	1.00	34.91
2954	O	CYS	B	892	-51.165	-2.775	19.71	1.00	35.02
2955	CB	CYS	B	892	-51.022	-3.733	22.637	1.00	32.86
2956	SG	CYS	B	892	-51.23	-2.055	23.225	1.00	33.36
2957	N	GLU	B	893	-53.169	-2.197	20.569	1.00	36.43
2958	CA	GLU	B	893	-53.364	-1.056	19.671	1.00	38.09
2959	C	GLU	B	893	-52.893	0.207	20.375	1.00	37.34

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TABLE 3

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

2960	O	GLU	B	893	-53.387	0.547	21.446	1.00	37.42
2961	CB	GLU	B	893	-54.839	-0.905	19.296	1.00	39.85
2962	CG	GLU	B	893	-55.466	-2.167	18.732	1.00	44.27
2963	CD	GLU	B	893	-56.859	-1.927	18.174	1.00	47.67
2964	OE1	GLU	B	893	-57.667	-1.257	18.856	1.00	48.57
2965	OE2	GLU	B	893	-57.148	-2.415	17.058	1.00	47.88
2966	N	HIS	B	894	-51.941	0.905	19.767	1.00	37.37
2967	CA	HIS	B	894	-51.385	2.116	20.358	1.00	37.13
2968	C	HIS	B	894	-51.031	3.139	19.281	1.00	38.33
2969	O	HIS	B	894	-50.287	2.84	18.346	1.00	36.79
2970	CB	HIS	B	894	-50.133	1.752	21.158	1.00	35.79
2971	CG	HIS	B	894	-49.58	2.872	21.98	1.00	35.87
2972	ND1	HIS	B	894	-50.169	3.298	23.152	1.00	36.46
2973	CD2	HIS	B	894	-48.466	3.627	21.824	1.00	35.59
2974	CE1	HIS	B	894	-49.439	4.261	23.685	1.00	35.97
2975	NE2	HIS	B	894	-48.4	4.48	22.899	1.00	35.75
2976	N	ARG	B	895	-51.581	4.344	19.418	1.00	40.55
2977	CA	ARG	B	895	-51.33	5.433	18.478	1.00	41.95
2978	C	ARG	B	895	-51.571	5.075	17.017	1.00	41.64
2979	O	ARG	B	895	-50.807	5.574	16.137	1.00	41.8
2980	CB	ARG	B	895	-49.891	5.936	18.615	1.00	45.81
2981	CG	ARG	B	895	-49.562	6.636	19.918	1.00	50.13
2982	CD	ARG	B	895	-48.13	7.141	19.863	1.00	55.44
2983	NE	ARG	B	895	-47.761	7.92	21.041	1.00	61.36
2984	CZ	ARG	B	895	-46.62	8.594	21.157	1.00	63.82
2985	NH1	ARG	B	895	-46.355	9.281	22.263	1.00	64.51
2986	NH2	ARG	B	895	-45.745	8.585	20.16	1.00	65.04
2987	N	GLY	B	896	-52.547	4.211	16.753	1.00	40.49
2988	CA	GLY	B	896	-52.84	3.838	15.38	1.00	39.34
2989	C	GLY	B	896	-51.993	2.699	14.844	1.00	39.16
2990	O	GLY	B	896	-52.191	2.231	13.717	1.00	39.56
2991	N	TYR	B	897	-51.033	2.254	15.641	1.00	37.54
2992	CA	TYR	B	897	-50.183	1.146	15.234	1.00	37.12
2993	C	TYR	B	897	-50.524	-0.072	16.09	1.00	35.49
2994	O	TYR	B	897	-50.817	0.062	17.28	1.00	34.93
2995	CB	TYR	B	897	-48.707	1.525	15.403	1.00	38.49
2996	CG	TYR	B	897	-48.196	2.505	14.363	1.00	39.36
2997	CD1	TYR	B	897	-47.832	2.074	13.086	1.00	39.37
2998	CD2	TYR	B	897	-48.082	3.865	14.654	1.00	39.39
2999	CE1	TYR	B	897	-47.365	2.973	12.125	1.00	40.88

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TABLE 3

STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

3000	CE2	TYR	B	897	-47.618	4.771	13.702	1.00	39.89
3001	CZ	TYR	B	897	-47.26	4.321	12.44	1.00	41.21
3002	OH	TYR	B	897	-46.782	5.214	11.502	1.00	41.62
3003	N	LEU	B	898	-50.522	-1.254	15.479	1.00	33.25
3004	CA	LEU	B	898	-50.816	-2.477	16.214	1.00	30.05
3005	C	LEU	B	898	-49.498	-3.12	16.614	1.00	28.4
3006	O	LEU	B	898	-48.672	-3.432	15.76	1.00	29.27
3007	CB	LEU	B	898	-51.608	-3.464	15.357	1.00	29.89
3008	CG	LEU	B	898	-51.932	-4.77	16.101	1.00	31.98
3009	CD1	LEU	B	898	-53.029	-4.504	17.111	1.00	31.19
3010	CD2	LEU	B	898	-52.366	-5.856	15.13	1.00	31.55
3011	N	TYR	B	899	-49.295	-3.306	17.911	1.00	25.31
3012	CA	TYR	B	899	-48.072	-3.921	18.397	1.00	23.61
3013	C	TYR	B	899	-48.313	-5.399	18.673	1.00	23.32
3014	O	TYR	B	899	-48.934	-5.772	19.669	1.00	23.81
3015	CB	TYR	B	899	-47.601	-3.208	19.657	1.00	21.28
3016	CG	TYR	B	899	-47.058	-1.824	19.383	1.00	20.94
3017	CD1	TYR	B	899	-45.692	-1.616	19.207	1.00	21.49
3018	CD2	TYR	B	899	-47.909	-0.719	19.303	1.00	20.98
3019	CE1	TYR	B	899	-45.183	-0.341	18.962	1.00	21.76
3020	CE2	TYR	B	899	-47.413	0.563	19.056	1.00	19.75
3021	CZ	TYR	B	899	-46.05	0.743	18.888	1.00	21.46
3022	OH	TYR	B	899	-45.546	1.998	18.647	1.00	22.37
3023	N	LEU	B	900	-47.813	-6.235	17.771	1.00	22.3
3024	CA	LEU	B	900	-47.977	-7.679	17.872	1.00	20.59
3025	C	LEU	B	900	-46.845	-8.341	18.659	1.00	18.95
3026	O	LEU	B	900	-45.658	-8.144	18.37	1.00	17.2
3027	CB	LEU	B	900	-48.052	-8.272	16.462	1.00	21.29
3028	CG	LEU	B	900	-48.382	-9.755	16.324	1.00	24.17
3029	CD1	LEU	B	900	-49.838	-10.004	16.748	1.00	22.19
3030	CD2	LEU	B	900	-48.156	-10.185	14.878	1.00	23.34
3031	N	ALA	B	901	-47.221	-9.119	19.667	1.00	17.56
3032	CA	ALA	B	901	-46.247	-9.825	20.492	1.00	17.89
3033	C	ALA	B	901	-46.078	-11.258	19.97	1.00	17.3
3034	O	ALA	B	901	-47.068	-11.943	19.697	1.00	16.11
3035	CB	ALA	B	901	-46.713	-9.847	21.948	1.00	18.18
3036	N	ILE	B	902	-44.827	-11.699	19.825	1.00	16.52
3037	CA	ILE	B	902	-44.533	-13.052	19.342	1.00	17.69
3038	C	ILE	B	902	-43.466	-13.72	20.211	1.00	18.83
3039	O	ILE	B	902	-42.837	-13.06	21.037	1.00	19.67

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

3040	CB	ILE	B	902	-44.035	-13.027	17.885	1.00	16.9
3041	CG1	ILE	B	902	-42.739	-12.216	17.792	1.00	17.07
3042	CG2	ILE	B	902	-45.112	-12.429	16.977	1.00	17.5
3043	CD1	ILE	B	902	-42.212	-12.052	16.375	1.00	16.46
3044	N	GLU	B	903	-43.263	-15.025	20.027	1.00	19.22
3045	CA	GLU	B	903	-42.262	-15.745	20.811	1.00	20.39
3046	C	GLU	B	903	-40.87	-15.22	20.514	1.00	20.17
3047	O	GLU	B	903	-40.529	-14.938	19.362	1.00	21.07
3048	CB	GLU	B	903	-42.271	-17.248	20.507	1.00	21.54
3049	CG	GLU	B	903	-43.446	-18.027	21.056	1.00	23.75
3050	CD	GLU	B	903	-43.382	-19.499	20.672	1.00	26.16
3051	OE1	GLU	B	903	-43.208	-19.803	19.471	1.00	25.39
3052	OE2	GLU	B	903	-43.511	-20.358	21.572	1.00	31.29
3053	N	TYR	B	904	-40.065	-15.097	21.56	1.00	18.31
3054	CA	TYR	B	904	-38.696	-14.64	21.405	1.00	19.78
3055	C	TYR	B	904	-37.804	-15.875	21.282	1.00	20.16
3056	O	TYR	B	904	-37.921	-16.808	22.078	1.00	20.69
3057	CB	TYR	B	904	-38.262	-13.802	22.619	1.00	17.65
3058	CG	TYR	B	904	-36.77	-13.58	22.694	1.00	16.21
3059	CD1	TYR	B	904	-36.105	-12.856	21.704	1.00	14.56
3060	CD2	TYR	B	904	-36.014	-14.119	23.739	1.00	18.55
3061	CE1	TYR	B	904	-34.73	-12.671	21.742	1.00	14.48
3062	CE2	TYR	B	904	-34.626	-13.94	23.792	1.00	18.34
3063	CZ	TYR	B	904	-33.995	-13.21	22.785	1.00	18.39
3064	OH	TYR	B	904	-32.635	-12.994	22.833	1.00	20.59
3065	N	ALA	B	905	-36.933	-15.877	20.275	1.00	20.53
3066	CA	ALA	B	905	-36.002	-16.981	20.042	1.00	21.54
3067	C	ALA	B	905	-34.632	-16.572	20.584	1.00	21.72
3068	O	ALA	B	905	-33.922	-15.778	19.96	1.00	22.8
3069	CB	ALA	B	905	-35.907	-17.28	18.553	1.00	20.39
3070	N	PRO	B	906	-34.242	-17.119	21.75	1.00	21.89
3071	CA	PRO	B	906	-32.964	-16.835	22.423	1.00	21.48
3072	C	PRO	B	906	-31.715	-17.159	21.608	1.00	21.95
3073	O	PRO	B	906	-30.64	-16.618	21.874	1.00	23.1
3074	CB	PRO	B	906	-33.023	-17.695	23.694	1.00	20.12
3075	CG	PRO	B	906	-34.494	-17.948	23.9	1.00	22.36
3076	CD	PRO	B	906	-35.011	-18.132	22.494	1.00	22.49
3077	N	HIS	B	907	-31.843	-18.041	20.624	1.00	20.52
3078	CA	HIS	B	907	-30.678	-18.426	19.844	1.00	20.22
3079	C	HIS	B	907	-30.641	-17.924	18.419	1.00	18.58



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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

3080	O	HIS	B	907	-29.855	-18.409	17.609	1.00	20.56
3081	CB	HIS	R	907	-30.538	-19.942	19.874	1.00	19.32
3082	CG	HIS	B	907	-30.498	-20.498	21.259	1.00	20.75
3083	ND1	HIS	B	907	-29.397	-20.371	22.079	1.00	21.25
3084	CD2	HIS	B	907	-31.441	-21.139	21.989	1.00	22.55
3085	CE1	HIS	B	907	-29.663	-20.912	23.255	1.00	23.11
3086	NE2	HIS	B	907	-30.897	-21.385	23.227	1.00	24.26
3087	N	GLY	B	908	-31.487	-16.95	18.111	1.00	17.74
3088	CA	GLY	B	908	-31.497	-16.392	16.772	1.00	15.17
3089	C	GLY	B	908	-31.946	-17.332	15.674	1.00	16.31
3090	O	GLY	B	908	-32.473	-18.423	15.936	1.00	15.41
3091	N	ASN	B	909	-31.727	-16.909	14.431	1.00	14.98
3092	CA	ASN	B	909	-32.138	-17.707	13.291	1.00	15.49
3093	C	ASN	B	909	-31.221	-18.915	13.1	1.00	15.27
3094	O	ASN	B	909	-30.049	-18.886	13.471	1.00	15.32
3095	CB	ASN	B	909	-32.188	-16.839	12.029	1.00	13.9
3096	CG	ASN	B	909	-30.816	-16.519	11.485	1.00	15.7
3097	OD1	ASN	B	909	-30.173	-17.359	10.846	1.00	15.2
3098	ND2	ASN	B	909	-30.354	-15.301	11.735	1.00	16.64
3099	N	LEU	B	910	-31.782	-19.979	12.531	1.00	15.29
3100	CA	LEU	B	910	-31.069	-21.229	12.297	1.00	14.11
3101	C	LEU	B	910	-29.798	-21.117	11.459	1.00	14.48
3102	O	LEU	B	910	-28.852	-21.863	11.679	1.00	14.9
3103	CB	LEU	B	910	-32.013	-22.245	11.645	1.00	12.32
3104	CG	LEU	B	910	-31.453	-23.638	11.352	1.00	10.53
3105	CD1	LEU	B	910	-30.921	-24.312	12.623	1.00	9.57
3106	CD2	LEU	B	910	-32.553	-24.462	10.757	1.00	10.7
3107	N	LEU	B	911	-29.768	-20.194	10.503	1.00	15.43
3108	CA	LEU	B	911	-28.59	-20.053	9.652	1.00	15.05
3109	C	LEU	B	911	-27.353	-19.587	10.4	1.00	15.4
3110	O	LEU	B	911	-26.287	-20.194	10.279	1.00	16.13
3111	CB	LEU	B	911	-28.873	-19.1	8.494	1.00	14.03
3112	CG	LEU	B	911	-27.771	-18.99	7.441	1.00	12.96
3113	CD1	LEU	B	911	-27.472	-20.368	6.845	1.00	13.72
3114	CD2	LEU	B	911	-28.211	-18.021	6.356	1.00	13.29
3115	N	ASP	B	912	-27.472	-18.504	11.161	1.00	16.78
3116	CA	ASP	B	912	-26.319	-18.021	11.909	1.00	19.24
3117	C	ASP	B	912	-25.925	-19.071	12.954	1.00	18.19
3118	O	ASP	B	912	-24.741	-19.259	13.252	1.00	16.71
3119	CB	ASP	B	912	-26.62	-16.679	12.594	1.00	23.79

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

3120	CG	ASP	B	912	-27.013	-15.578	11.602	1.00	31.22
3121	OD1	ASP	B	912	-26.442	-15.516	10.484	1.00	34.44
3122	OD2	ASP	B	912	-27.892	-14.756	11.946	1.00	33.85
3123	N	PHE	B	913	-26.92	-19.776	13.486	1.00	17.09
3124	CA	PHE	B	913	-26.665	-20.79	14.497	1.00	16.9
3125	C	PHE	B	913	-25.84	-21.937	13.911	1.00	16.77
3126	O	PHE	B	913	-24.899	-22.421	14.539	1.00	16.95
3127	CB	PHE	B	913	-27.99	-21.315	15.074	1.00	17.67
3128	CG	PHE	B	913	-27.841	-21.975	16.424	1.00	18.62
3129	CD1	PHE	B	913	-27.452	-21.229	17.536	1.00	17.89
3130	CD2	PHE	B	913	-28.048	-23.347	16.576	1.00	17.79
3131	CE1	PHE	B	913	-27.265	-21.838	18.785	1.00	18.55
3132	CE2	PHE	B	913	-27.865	-23.967	17.822	1.00	19.04
3133	CZ	PHE	B	913	-27.473	-23.21	18.926	1.00	18.44
3134	N	LEU	B	914	-26.189	-22.365	12.701	1.00	16.7
3135	CA	LEU	B	914	-25.463	-23.438	12.031	1.00	16.24
3136	C	LEU	B	914	-24.022	-23.012	11.758	1.00	16.84
3137	O	LEU	B	914	-23.068	-23.753	12.031	1.00	15.02
3138	CB	LEU	B	914	-26.151	-23.79	10.709	1.00	13.93
3139	CG	LEU	B	914	-27.501	-24.501	10.841	1.00	13.94
3140	CD1	LEU	B	914	-28.193	-24.569	9.484	1.00	9.64
3141	CD2	LEU	B	914	-27.276	-25.895	11.425	1.00	8.9
3142	N	ARG	B	915	-23.869	-21.806	11.22	1.00	17.09
3143	CA	ARG	B	915	-22.545	-21.285	10.905	1.00	17.59
3144	C	ARG	B	915	-21.693	-21.041	12.155	1.00	18.06
3145	O	ARG	B	915	-20.487	-21.276	12.142	1.00	15.64
3146	CB	ARG	B	915	-22.687	-20.006	10.073	1.00	17.12
3147	CG	ARG	B	915	-23.237	-20.284	8.676	1.00	19.7
3148	CD	ARG	B	915	-23.449	-19.026	7.851	1.00	18.64
3149	NE	ARG	B	915	-23.905	-19.352	6.502	1.00	19.64
3150	CZ	ARG	B	915	-24.225	-18.452	5.574	1.00	19.16
3151	NH1	ARG	B	915	-24.623	-18.851	4.374	1.00	18.16
3152	NH2	ARG	B	915	-24.151	-17.157	5.846	1.00	19.48
3153	N	LYS	B	916	-22.321	-20.582	13.236	1.00	19.74
3154	CA	LYS	B	916	-21.587	-20.328	14.472	1.00	20.88
3155	C	LYS	B	916	-21.129	-21.631	15.103	1.00	20.68
3156	O	LYS	B	916	-20.243	-21.626	15.949	1.00	21.2
3157	CB	LYS	B	916	-22.45	-19.563	15.48	1.00	22.11
3158	CG	LYS	B	916	-22.621	-18.088	15.185	1.00	25.47
3159	CD	LYS	B	916	-23.492	-17.438	16.255	1.00	29.88

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

3160	CE	LYS	B	916	-23.799	-15.984	15.926	1.00	32.63
3161	NZ	LYS	B	916	-22.551	-15.197	15.725	1.00	34.08
3162	N	SER	B	917	-21.738	-22.742	14.696	1.00	20.38
3163	CA	SER	B	917	-21.38	-24.051	15.236	1.00	20.19
3164	C	SER	B	917	-20.116	-24.628	14.587	1.00	20.72
3165	O	SER	B	917	-19.622	-25.68	15.007	1.00	20.91
3166	CB	SER	B	917	-22.525	-25.044	15.034	1.00	21.01
3167	OG	SER	B	917	-22.432	-25.675	13.761	1.00	20.22
3168	N	ARG	B	918	-19.609	-23.957	13.555	1.00	20.12
3169	CA	ARG	B	918	-18.404	-24.415	12.861	1.00	20.15
3170	C	ARG	B	918	-17.165	-24.185	13.734	1.00	21.15
3171	O	ARG	B	918	-16.291	-23.386	13.401	1.00	20.68
3172	CB	ARG	B	918	-18.254	-23.673	11.533	1.00	18.24
3173	CG	ARG	B	918	-19.308	-24.032	10.509	1.00	16.45
3174	CD	ARG	B	918	-18.991	-23.433	9.152	1.00	14.73
3175	NE	ARG	B	918	-19.951	-23.872	8.147	1.00	14.41
3176	CZ	ARG	B	918	-19.806	-23.701	6.838	1.00	14.25
3177	NH1	ARG	B	918	-20.742	-24.14	6.007	1.00	15.52
3178	NH2	ARG	B	918	-18.728	-23.101	6.355	1.00	14.64
3179	N	VAL	B	919	-17.103	-24.901	14.852	1.00	22.76
3180	CA	VAL	B	919	-16.01	-24.769	15.805	1.00	24.37
3181	C	VAL	B	919	-14.634	-24.949	15.172	1.00	25.11
3182	O	VAL	B	919	-13.657	-24.347	15.612	1.00	23.74
3183	CB	VAL	B	919	-16.183	-25.772	16.977	1.00	25.19
3184	CG1	VAL	B	919	-15.985	-27.2	16.487	1.00	24.27
3185	CG2	VAL	B	919	-15.219	-25.433	18.093	1.00	25.97
3186	N	LEU	B	920	-14.559	-25.76	14.124	1.00	27.34
3187	CA	LEU	B	920	-13.289	-25.992	13.449	1.00	28.69
3188	C	LEU	B	920	-12.754	-24.688	12.867	1.00	31.11
3189	O	LEU	B	920	-11.688	-24.654	12.256	1.00	33.34
3190	CB	LEU	B	920	-13.462	-27.035	12.344	1.00	25.61
3191	CG	LEU	B	920	-12.201	-27.465	11.593	1.00	24.93
3192	CD1	LEU	B	920	-11.137	-27.925	12.583	1.00	22.75
3193	CD2	LEU	B	920	-12.554	-28.58	10.612	1.00	21.83
3194	N	GLU	B	921	-13.498	-23.608	13.064	1.00	33.58
3195	CA	GLU	B	921	-13.074	-22.315	12.561	1.00	35.96
3196	C	GLU	B	921	-13.175	-21.244	13.64	1.00	35.57
3197	O	GLU	B	921	-12.351	-20.337	13.705	1.00	36.22
3198	CB	GLU	B	921	-13.914	-21.909	11.362	1.00	39.74
3199	CG	GLU	B	921	-13.165	-20.998	10.43	1.00	46.25

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

3200	CD	GLU	B	921	-14.068	-20.314	9.444	1.00	50.91
3201	OE1	GLU	B	921	-14.866	-19.457	9.886	1.00	55.65
3202	OE2	GLU	B	921	-13.978	-20.64	8.236	1.00	53.11
3203	N	THR	B	922	-14.187	-21.349	14.49	1.00	34.96
3204	CA	THR	B	922	-14.358	-20.381	15.564	1.00	34.08
3205	C	THR	B	922	-13.397	-20.687	16.705	1.00	33.88
3206	O	THR	B	922	-12.994	-19.788	17.441	1.00	35.18
3207	CB	THR	B	922	-15.793	-20.402	16.107	1.00	33.59
3208	OG1	THR	B	922	-16.112	-21.726	16.554	1.00	33.43
3209	CG2	THR	B	922	-16.776	-19.981	15.024	1.00	32.41
3210	N	ASP	B	923	-13.021	-21.958	16.836	1.00	33.6
3211	CA	ASP	B	923	-12.11	-22.401	17.892	1.00	32.63
3212	C	ASP	B	923	-11.508	-23.762	17.531	1.00	30.92
3213	O	ASP	B	923	-11.912	-24.794	18.063	1.00	29.86
3214	CB	ASP	B	923	-12.875	-22.485	19.215	1.00	34.95
3215	CG	ASP	B	923	-12.029	-23.015	20.355	1.00	37.18
3216	OD1	ASP	B	923	-10.777	-22.935	20.281	1.00	37.37
3217	OD2	ASP	B	923	-12.631	-23.498	21.338	1.00	37.74
3218	N	PRO	B	924	-10.52	-23.77	16.62	1.00	29.72
3219	CA	PRO	B	924	-9.842	-24.986	16.154	1.00	29.24
3220	C	PRO	B	924	-9.2	-25.885	17.209	1.00	29.03
3221	O	PRO	B	924	-9.071	-27.087	17	1.00	28.51
3222	CB	PRO	B	924	-8.831	-24.45	15.141	1.00	28.98
3223	CG	PRO	B	924	-8.563	-23.052	15.625	1.00	28.6
3224	CD	PRO	B	924	-9.923	-22.569	16.01	1.00	28.11
3225	N	ALA	B	925	-8.8	-25.319	18.341	1.00	29.84
3226	CA	ALA	B	925	-8.185	-26.128	19.389	1.00	29.56
3227	C	ALA	B	925	-9.222	-27.081	19.977	1.00	30.22
3228	O	ALA	B	925	-8.944	-28.26	20.213	1.00	30.54
3229	CB	ALA	B	925	-7.619	-25.232	20.476	1.00	28.53
3230	N	PHE	B	926	-10.42	-26.557	20.209	1.00	30.36
3231	CA	PHE	B	926	-11.517	-27.344	20.76	1.00	31.73
3232	C	PHE	B	926	-11.89	-28.439	19.766	1.00	31.74
3233	O	PHE	B	926	-12.042	-29.611	20.131	1.00	32.83
3234	CB	PHE	B	926	-12.733	-26.439	21.011	1.00	33.34
3235	CG	PHE	B	926	-13.913	-27.15	21.619	1.00	35.38
3236	CD1	PHE	B	926	-13.881	-27.581	22.943	1.00	35.26
3237	CD2	PHE	B	926	-15.059	-27.392	20.866	1.00	36.04
3238	CE1	PHE	B	926	-14.972	-28.242	23.509	1.00	34.92
3239	CE2	PHE	B	926	-16.156	-28.053	21.424	1.00	36.73

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

3240	CZ	PHE	B	926	-16.111	-28.479	22.75	1.00	34.62
3241	N	ALA	B	927	-12.032	-28.042	18.505	1.00	29.09
3242	CA	ALA	B	927	-12.387	-28.97	17.444	1.00	27.13
3243	C	ALA	B	927	-11.4	-30.13	17.381	1.00	26.78
3244	O	ALA	B	927	-11.796	-31.294	17.367	1.00	25.73
3245	CB	ALA	B	927	-12.425	-28.237	16.105	1.00	25.92
3246	N	ILE	B	928	-10.112	-29.804	17.343	1.00	27.44
3247	CA	ILE	B	928	-9.068	-30.82	17.266	1.00	27.88
3248	C	ILE	B	928	-9.064	-31.713	18.493	1.00	28.48
3249	O	ILE	B	928	-8.877	-32.928	18.39	1.00	28.86
3250	CB	ILE	B	928	-7.669	-30.183	17.128	1.00	27.42
3251	CG1	ILE	B	928	-7.555	-29.464	15.779	1.00	27.19
3252	CG2	ILE	B	928	-6.591	-31.257	17.267	1.00	27.42
3253	CD1	ILE	B	928	-7.836	-30.348	14.593	1.00	26.28
3254	N	ALA	B	929	-9.271	-31.103	19.653	1.00	26.62
3255	CA	ALA	B	929	-9.283	-31.843	20.896	1.00	26.92
3256	C	ALA	B	929	-10.462	-32.799	20.934	1.00	27.42
3257	O	ALA	B	929	-10.336	-33.945	21.369	1.00	27.09
3258	CB	ALA	B	929	-9.355	-30.878	22.071	1.00	27.81
3259	N	ASN	B	930	-11.609	-32.331	20.461	1.00	27.17
3260	CA	ASN	B	930	-12.806	-33.148	20.478	1.00	26.31
3261	C	ASN	B	930	-13.086	-33.901	19.188	1.00	26.63
3262	O	ASN	B	930	-14.095	-34.602	19.084	1.00	26.43
3263	CB	ASN	B	930	-13.985	-32.273	20.865	1.00	27.74
3264	CG	ASN	B	930	-13.821	-31.687	22.248	1.00	29.39
3265	OD1	ASN	B	930	-14.093	-32.348	23.244	1.00	30.65
3266	ND2	ASN	B	930	-13.343	-30.45	22.319	1.00	31.19
3267	N	SER	B	931	-12.189	-33.764	18.214	1.00	25.53
3268	CA	SER	B	931	-12.33	-34.448	16.93	1.00	24.84
3269	C	SER	B	931	-13.672	-34.136	16.263	1.00	23.36
3270	O	SER	B	931	-14.256	-34.981	15.577	1.00	23.18
3271	CB	SER	B	931	-12.198	-35.961	17.135	1.00	25.46
3272	OG	SER	B	931	-10.964	-36.287	17.756	1.00	26.86
3273	N	THR	B	932	-14.154	-32.916	16.455	1.00	20.95
3274	CA	THR	B	932	-15.431	-32.525	15.881	1.00	20.71
3275	C	THR	B	932	-15.305	-31.332	14.934	1.00	18.2
3276	O	THR	B	932	-14.305	-30.624	14.946	1.00	18.6
3277	CB	THR	B	932	-16.442	-32.184	16.996	1.00	20.5
3278	OG1	THR	B	932	-17.734	-31.977	16.418	1.00	24.1
3279	CG2	THR	B	932	-16.011	-30.93	17.747	1.00	19.12

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TABLE 3

STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

3280	N	ALA	B	933	-16.322	-31.126	14.109	1.00	16.55
3281	CA	ALA	F	933	-16.33	-30.017	13.159	1.00	16.69
3282	C	ALA	B	933	-17.495	-29.101	13.507	1.00	16.4
3283	O	ALA	B	933	-17.718	-28.077	12.859	1.00	15.9
3284	CB	ALA	B	933	-16.478	-30.541	11.724	1.00	14
3285	N	SER	B	934	-18.238	-29.483	14.54	1.00	15.33
3286	CA	SER	B	934	-19.382	-28.7	14.974	1.00	16.21
3287	C	SER	B	934	-19.759	-28.95	16.434	1.00	15.97
3288	O	SER	B	934	-19.544	-30.039	16.967	1.00	15.17
3289	CB	SER	B	934	-20.589	-29.002	14.081	1.00	14.52
3290	OG	SER	B	934	-21.735	-28.313	14.544	1.00	14.24
3291	N	THR	B	935	-20.317	-27.93	17.075	1.00	15.47
3292	CA	THR	B	935	-20.755	-28.064	18.455	1.00	15.83
3293	C	THR	B	935	-22.076	-28.804	18.431	1.00	15.38
3294	O	THR	B	935	-22.602	-29.188	19.472	1.00	16.53
3295	CB	THR	B	935	-20.991	-26.694	19.11	1.00	16.74
3296	OG1	THR	B	935	-21.759	-25.876	18.221	1.00	16.85
3297	CG2	THR	B	935	-19.658	-26.007	19.432	1.00	15.91
3298	N	LEU	B	936	-22.605	-29.003	17.226	1.00	15.46
3299	CA	LEU	B	936	-23.886	-29.679	17.037	1.00	14.4
3300	C	LEU	B	936	-23.712	-31.117	16.575	1.00	15.25
3301	O	LEU	B	936	-22.894	-31.399	15.702	1.00	16.9
3302	CB	LEU	B	936	-24.728	-28.911	16.014	1.00	12.24
3303	CG	LEU	B	936	-25.142	-27.475	16.362	1.00	12.48
3304	CD1	LEU	B	936	-25.646	-26.743	15.113	1.00	8.83
3305	CD2	LEU	B	936	-26.212	-27.517	17.448	1.00	8.71
3306	N	SER	B	937	-24.494	-32.025	17.151	1.00	16.04
3307	CA	SER	B	937	-24.418	-33.436	16.783	1.00	16.47
3308	C	SER	B	937	-25.327	-33.778	15.601	1.00	16.56
3309	O	SER	B	937	-26.187	-32.988	15.21	1.00	16.15
3310	CB	SER	B	937	-24.803	-34.316	17.977	1.00	17.2
3311	OG	SER	B	937	-26.197	-34.246	18.256	1.00	19.93
3312	N	SER	B	938	-25.124	-34.964	15.037	1.00	16.03
3313	CA	SER	B	938	-25.932	-35.446	13.927	1.00	16.15
3314	C	SER	B	938	-27.409	-35.465	14.344	1.00	16.88
3315	O	SER	B	938	-28.294	-35.068	13.575	1.00	15.32
3316	CB	SER	B	938	-25.486	-36.862	13.546	1.00	16.4
3317	OG	SER	B	938	-26.311	-37.41	12.536	1.00	15.54
3318	N	GLN	B	939	-27.663	-35.931	15.567	1.00	17.27
3319	CA	GLN	B	939	-29.026	-36.008	16.096	1.00	18.82

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

3320	C	GLN	B	939	-29.674	-34.635	16.201	1.00	18.23
3321	O	GLN	B	939	-30.817	-34.444	15.785	1.00	18.64
3322	CB	GLN	B	939	-29.04	-36.666	17.484	1.00	18.42
3323	CG	GLN	B	939	-28.998	-38.176	17.469	1.00	22.33
3324	CD	GLN	B	939	-30.273	-38.796	16.922	1.00	23.23
3325	OE1	GLN	B	939	-30.273	-39.41	15.854	1.00	22.12
3326	NE2	GLN	B	939	-31.368	-38.637	17.658	1.00	22.95
3327	N	GLN	B	940	-28.947	-33.682	16.774	1.00	16.62
3328	CA	GLN	B	940	-29.481	-32.341	16.927	1.00	16.77
3329	C	GLN	B	940	-29.788	-31.759	15.559	1.00	15.18
3330	O	GLN	B	940	-30.799	-31.087	15.378	1.00	16.65
3331	CB	GLN	B	940	-28.487	-31.457	17.682	1.00	18.95
3332	CG	GLN	B	940	-28.25	-31.906	19.118	1.00	20.7
3333	CD	GLN	B	940	-27.226	-31.048	19.829	1.00	23.39
3334	OE1	GLN	B	940	-26.07	-30.974	19.416	1.00	26.95
3335	NE2	GLN	B	940	-27.645	-30.389	20.904	1.00	25.06
3336	N	LEU	B	941	-28.922	-32.028	14.589	1.00	14.4
3337	CA	LEU	B	941	-29.141	-31.524	13.242	1.00	13.82
3338	C	LEU	B	941	-30.401	-32.154	12.648	1.00	13.73
3339	O	LEU	B	941	-31.224	-31.452	12.055	1.00	13.91
3340	CB	LEU	B	941	-27.911	-31.786	12.357	1.00	11.58
3341	CG	LEU	B	941	-26.636	-31.021	12.789	1.00	12.38
3342	CD1	LEU	B	941	-25.488	-31.35	11.85	1.00	10.03
3343	CD2	LEU	B	941	-26.886	-29.518	12.785	1.00	6.79
3344	N	LEU	B	942	-30.581	-33.462	12.828	1.00	13.41
3345	CA	LEU	B	942	-31.777	-34.107	12.29	1.00	13.64
3346	C	LEU	B	942	-33.035	-33.607	12.995	1.00	12.98
3347	O	LEU	B	942	-34.069	-33.428	12.347	1.00	11.72
3348	CB	LEU	B	942	-31.687	-35.634	12.398	1.00	15.59
3349	CG	LEU	B	942	-30.757	-36.384	11.431	1.00	16.47
3350	CD1	LEU	B	942	-30.94	-37.882	11.641	1.00	17.56
3351	CD2	LEU	B	942	-31.063	-36.027	9.986	1.00	15.21
3352	N	HIS	B	943	-32.949	-33.38	14.312	1.00	12.35
3353	CA	HIS	B	943	-34.085	-32.86	15.084	1.00	11.54
3354	C	HIS	B	943	-34.527	-31.488	14.564	1.00	10.89
3355	O	HIS	B	943	-35.715	-31.167	14.569	1.00	10.75
3356	CB	HIS	B	943	-33.736	-32.744	16.574	1.00	14.15
3357	CG	HIS	B	943	-33.904	-34.023	17.331	1.00	15.52
3358	ND1	HIS	B	943	-35.099	-34.71	17.373	1.00	15.95
3359	CD2	HIS	B	943	-33.02	-34.761	18.042	1.00	14.78

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

3360	CE1	HIS	B	943	-34.942	-35.819	18.072	1.00	16.93
3361	NE2	HIS	B	943	-33.69	-35.875	18.488	1.00	17.45
3362	N	PHE	B	944	-33.57	-30.672	14.138	1.00	11.3
3363	CA	PHE	B	944	-33.896	-29.362	13.571	1.00	12.84
3364	C	PHE	B	944	-34.747	-29.607	12.318	1.00	11.7
3365	O	PHE	B	944	-35.782	-28.975	12.132	1.00	10.51
3366	CB	PHE	B	944	-32.616	-28.607	13.183	1.00	14.43
3367	CG	PHE	B	944	-31.903	-27.959	14.345	1.00	14.41
3368	CD1	PHE	B	944	-30.528	-27.765	14.305	1.00	14.78
3369	CD2	PHE	B	944	-32.613	-27.485	15.445	1.00	16.6
3370	CE1	PHE	B	944	-29.866	-27.107	15.336	1.00	15.88
3371	CE2	PHE	B	944	-31.961	-26.823	16.488	1.00	15.89
3372	CZ	PHE	B	944	-30.585	-26.634	16.431	1.00	18.13
3373	N	ALA	B	945	-34.317	-30.549	11.477	1.00	12.38
3374	CA	ALA	B	945	-35.048	-30.873	10.248	1.00	12.5
3375	C	ALA	B	945	-36.432	-31.423	10.547	1.00	12.75
3376	O	ALA	B	945	-37.403	-31.051	9.886	1.00	13.3
3377	CB	ALA	B	945	-34.261	-31.882	9.403	1.00	11.68
3378	N	ALA	B	946	-36.527	-32.306	11.54	1.00	13.34
3379	CA	ALA	B	946	-37.815	-32.892	11.915	1.00	12.97
3380	C	ALA	B	946	-38.719	-31.807	12.491	1.00	12.61
3381	O	ALA	B	946	-39.928	-31.811	12.26	1.00	12.06
3382	CB	ALA	B	946	-37.621	-34.022	12.935	1.00	10.15
3383	N	ASP	B	947	-38.13	-30.877	13.238	1.00	13.34
3384	CA	ASP	B	947	-38.896	-29.769	13.82	1.00	14.64
3385	C	ASP	B	947	-39.58	-28.964	12.721	1.00	13.91
3386	O	ASP	B	947	-40.778	-28.705	12.791	1.00	14.2
3387	CB	ASP	B	947	-37.98	-28.831	14.624	1.00	15.83
3388	CG	ASP	B	947	-37.733	-29.321	16.045	1.00	16.46
3389	OD1	ASP	B	947	-36.953	-28.663	16.766	1.00	18.77
3390	OD2	ASP	B	947	-38.319	-30.35	16.447	1.00	18
3391	N	VAL	B	948	-38.813	-28.568	11.706	1.00	13.09
3392	CA	VAL	B	948	-39.269	-27.793	10.601	1.00	13.51
3393	C	VAL	B	948	-40.402	-28.599	9.801	1.00	12.83
3394	O	VAL	B	948	-41.444	-28.062	9.409	1.00	11.74
3395	CB	VAL	B	948	-38.255	-27.279	9.65	1.00	13.8
3396	CG1	VAL	B	948	-38.879	-26.559	8.461	1.00	10.78
3397	CG2	VAL	B	948	-37.325	-26.33	10.402	1.00	12.37
3398	N	ALA	B	949	-40.125	-29.878	9.553	1.00	11.07
3399	CA	ALA	B	949	-41.086	-30.702	8.822	1.00	10.95



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TABLE 3

STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

3400	C	ALA	B	949	-42.384	-30.809	9.64	1.00	10.27
3401	O	ALA	B	949	-43.476	-30.737	9.086	1.00	11.55
3402	CB	ALA	B	949	-40.501	-32.113	8.544	1.00	9.65
3403	N	ARG	B	950	-42.264	-30.962	10.956	1.00	7.63
3404	CA	ARG	B	950	-43.438	-31.068	11.817	1.00	8.24
3405	C	ARG	B	950	-44.241	-29.771	11.767	1.00	8.88
3406	O	ARG	B	950	-45.466	-29.797	11.669	1.00	11.99
3407	CB	ARG	B	950	-43.024	-31.37	13.274	1.00	9.15
3408	CG	ARG	B	950	-44.194	-31.725	14.19	1.00	9.55
3409	CD	ARG	B	950	-43.754	-32.087	15.597	1.00	10
3410	NE	ARG	B	950	-42.65	-33.044	15.597	1.00	13.36
3411	CZ	ARG	B	950	-41.376	-32.73	15.829	1.00	14.6
3412	NH1	ARG	B	950	-40.445	-33.677	15.795	1.00	15.48
3413	NH2	ARG	B	950	-41.028	-31.477	16.108	1.00	12.45
3414	N	GLY	B	951	-43.549	-28.639	11.842	1.00	9.41
3415	CA	GLY	B	951	-44.224	-27.354	11.784	1.00	10.64
3416	C	GLY	B	951	-44.865	-27.119	10.428	1.00	12.49
3417	O	GLY	B	951	-45.959	-26.549	10.334	1.00	11.05
3418	N	MET	B	952	-44.199	-27.56	9.363	1.00	13.41
3419	CA	MET	B	952	-44.768	-27.376	8.029	1.00	15.12
3420	C	MET	B	952	-45.962	-28.305	7.791	1.00	15.99
3421	O	MET	B	952	-46.879	-27.967	7.036	1.00	15.41
3422	CB	MET	B	952	-43.704	-27.579	6.955	1.00	12.57
3423	CG	MET	B	952	-42.748	-26.407	6.844	1.00	14.09
3424	SD	MET	B	952	-43.638	-24.842	6.626	1.00	17.27
3425	CE	MET	B	952	-44.371	-25.082	4.98	1.00	14.18
3426	N	ASP	B	953	-45.959	-29.47	8.433	1.00	16.21
3427	CA	ASP	B	953	-47.081	-30.392	8.286	1.00	15.95
3428	C	ASP	B	953	-48.278	-29.648	8.856	1.00	16.48
3429	O	ASP	B	953	-49.33	-29.528	8.226	1.00	13.81
3430	CB	ASP	B	953	-46.853	-31.657	9.106	1.00	17.37
3431	CG	ASP	B	953	-48.02	-32.626	9.015	1.00	18.03
3432	OD1	ASP	B	953	-48.379	-33.226	10.051	1.00	21.62
3433	OD2	ASP	B	953	-48.572	-32.797	7.911	1.00	16.54
3434	N	TYR	B	954	-48.089	-29.131	10.064	1.00	15.64
3435	CA	TYR	B	954	-49.125	-28.386	10.738	1.00	15.19
3436	C	TYR	B	954	-49.627	-27.223	9.88	1.00	14.75
3437	O	TYR	B	954	-50.832	-27.068	9.691	1.00	16.67
3438	CB	TYR	B	954	-48.596	-27.873	12.075	1.00	15.2
3439	CG	TYR	B	954	-49.53	-26.922	12.783	1.00	14.79

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

3440	CD1	TYR	B	954	-50.626	-27.394	13.514	1.00	15
3441	CD2	TYR	B	954	-49.332	-25.546	12.706	1.00	13.58
3442	CE1	TYR	B	954	-51.506	-26.508	14.153	1.00	15.31
3443	CE2	TYR	B	954	-50.202	-24.652	13.338	1.00	15.59
3444	CZ	TYR	B	954	-51.286	-25.139	14.056	1.00	15.77
3445	OH	TYR	B	954	-52.152	-24.251	14.649	1.00	16.39
3446	N	LEU	B	955	-48.716	-26.412	9.347	1.00	14.48
3447	CA	LEU	B	955	-49.128	-25.269	8.53	1.00	13.67
3448	C	LEU	B	955	-49.77	-25.612	7.185	1.00	13.98
3449	O	LEU	B	955	-50.776	-25.007	6.804	1.00	12.33
3450	CB	LEU	B	955	-47.951	-24.322	8.303	1.00	13.23
3451	CG	LEU	B	955	-47.415	-23.609	9.547	1.00	12.75
3452	CD1	LEU	B	955	-46.251	-22.71	9.16	1.00	7.99
3453	CD2	LEU	B	955	-48.532	-22.801	10.194	1.00	13.51
3454	N	SER	B	956	-49.201	-26.573	6.465	1.00	14.69
3455	CA	SER	B	956	-49.758	-26.95	5.169	1.00	16.95
3456	C	SER	B	956	-51.134	-27.594	5.304	1.00	18.64
3457	O	SER	B	956	-51.974	-27.465	4.407	1.00	18.89
3458	CB	SER	B	956	-48.805	-27.89	4.413	1.00	16.17
3459	OG	SER	B	956	-48.377	-28.971	5.219	1.00	22.19
3460	N	GLN	B	957	-51.367	-28.278	6.423	1.00	19.82
3461	CA	GLN	B	957	-52.654	-28.926	6.669	1.00	22.04
3462	C	GLN	B	957	-53.695	-27.857	6.946	1.00	20.53
3463	O	GLN	B	957	-54.89	-28.096	6.835	1.00	19.31
3464	CB	GLN	B	957	-52.568	-29.887	7.867	1.00	27.91
3465	CG	GLN	B	957	-51.793	-31.161	7.588	1.00	33.69
3466	CD	GLN	B	957	-52.594	-32.165	6.782	1.00	40.39
3467	OE1	GLN	B	957	-53.216	-33.073	7.342	1.00	42.88
3468	NE2	GLN	B	957	-52.597	-32.001	5.459	1.00	43.57
3469	N	LYS	B	958	-53.228	-26.674	7.314	1.00	21.32
3470	CA	LYS	B	958	-54.122	-25.562	7.587	1.00	21.98
3471	C	LYS	B	958	-54.129	-24.641	6.373	1.00	23.35
3472	O	LYS	B	958	-54.515	-23.476	6.468	1.00	25.76
3473	CB	LYS	B	958	-53.66	-24.797	8.83	1.00	23.93
3474	CG	LYS	B	958	-53.553	-25.655	10.094	1.00	22.27
3475	CD	LYS	B	958	-54.596	-25.284	11.112	1.00	22.2
3476	CE	LYS	B	958	-54.396	-23.866	11.623	1.00	23.18
3477	NZ	LYS	B	958	-55.505	-23.461	12.542	1.00	23.54
3478	N	GLN	B	959	-53.672	-25.167	5.238	1.00	23.09
3479	CA	GLN	B	959	-53.655	-24.429	3.977	1.00	24.4

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

3480	C	GLN	B	959	-52.572	-23.359	3.817	1.00	23.63
3481	O	GLN	B	959	-52.482	-22.723	2.764	1.00	25.21
3482	CB	GLN	B	959	-55.019	-23.776	3.733	1.00	27.57
3483	CG	GLN	B	959	-56.209	-24.715	3.823	1.00	33.43
3484	CD	GLN	B	959	-56.133	-25.841	2.814	1.00	38.54
3485	OE1	GLN	B	959	-55.854	-26.989	3.168	1.00	41.98
3486	NE2	GLN	B	959	-56.373	-25.517	1.543	1.00	40.11
3487	N	PHE	B	960	-51.76	-23.138	4.84	1.00	20.46
3488	CA	PHE	B	960	-50.722	-22.134	4.718	1.00	18.83
3489	C	PHE	B	960	-49.681	-22.493	3.664	1.00	17.89
3490	O	PHE	B	960	-49.316	-23.661	3.499	1.00	17.05
3491	CB	PHE	B	960	-50.006	-21.915	6.052	1.00	19.29
3492	CG	PHE	B	960	-50.8	-21.127	7.046	1.00	19.67
3493	CD1	PHE	B	960	-51.767	-21.74	7.83	1.00	19.53
3494	CD2	PHE	B	960	-50.58	-19.76	7.196	1.00	20.28
3495	CE1	PHE	B	960	-52.507	-21.008	8.754	1.00	19.62
3496	CE2	PHE	B	960	-51.312	-19.016	8.116	1.00	20
3497	CZ	PHE	B	960	-52.279	-19.642	8.897	1.00	20.16
3498	N	ILE	B	961	-49.218	-21.466	2.954	1.00	16.2
3499	CA	ILE	B	961	-48.184	-21.6	1.936	1.00	15.28
3500	C	ILE	B	961	-47.138	-20.582	2.384	1.00	15.43
3501	O	ILE	B	961	-47.424	-19.388	2.482	1.00	15.71
3502	CB	ILE	B	961	-48.709	-21.247	0.515	1.00	14.3
3503	CG1	ILE	B	961	-49.854	-22.19	0.128	1.00	11.91
3504	CG2	ILE	B	961	-47.585	-21.376	-0.511	1.00	11.17
3505	CD1	ILE	B	961	-50.485	-21.88	-1.24	1.00	10.39
3506	N	HIS	B	962	-45.932	-21.064	2.666	1.00	15.37
3507	CA	HIS	B	962	-44.856	-20.217	3.164	1.00	14.86
3508	C	HIS	B	962	-44.177	-19.328	2.113	1.00	16.12
3509	O	HIS	B	962	-44.055	-18.116	2.314	1.00	16.81
3510	CB	HIS	B	962	-43.831	-21.099	3.883	1.00	11.98
3511	CG	HIS	B	962	-42.885	-20.339	4.755	1.00	10.98
3512	ND1	HIS	B	962	-41.915	-19.5	4.249	1.00	9.34
3513	CD2	HIS	B	962	-42.761	-20.29	6.103	1.00	9.6
3514	CE1	HIS	B	962	-41.232	-18.97	5.248	1.00	9.64
3515	NE2	HIS	B	962	-41.727	-19.431	6.383	1.00	10.59
3516	N	ARG	B	963	-43.732	-19.926	1.007	1.00	17.43
3517	CA	ARG	B	963	-43.081	-19.201	-0.098	1.00	18.42
3518	C	ARG	B	963	-41.585	-18.902	0.076	1.00	18.48
3519	O	ARG	B	963	-40.868	-18.746	-0.909	1.00	18.71

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TABLE 3

STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

3520	CB	ARG	B	963	-43.782	-17.852	-0.392	1.00	19.56
3521	CG	ARG	B	963	-45.282	-17.884	-0.705	1.00	19.85
3522	CD	ARG	B	963	-45.73	-16.555	-1.348	1.00	20.3
3523	NE	ARG	B	963	-45.189	-15.386	-0.652	1.00	25.89
3524	CZ	ARG	B	963	-45.627	-14.93	0.524	1.00	28.08
3525	NH1	ARG	B	963	-46.634	-15.526	1.152	1.00	27.08
3526	NH2	ARG	B	963	-45.026	-13.898	1.099	1.00	28.42
3527	N	ASP	B	964	-41.111	-18.815	1.313	1.00	18.97
3528	CA	ASP	B	964	-39.706	-18.489	1.547	1.00	20.1
3529	C	ASP	B	964	-39.07	-19.339	2.649	1.00	19.72
3530	O	ASP	B	964	-38.378	-18.827	3.535	1.00	18.34
3531	CB	ASP	B	964	-39.601	-16.992	1.882	1.00	23.03
3532	CG	ASP	B	964	-38.166	-16.496	1.954	1.00	26.5
3533	OD1	ASP	B	964	-37.311	-17.008	1.206	1.00	24.46
3534	OD2	ASP	B	964	-37.898	-15.57	2.753	1.00	30.55
3535	N	LEU	B	965	-39.295	-20.645	2.574	1.00	17.81
3536	CA	LEU	B	965	-38.763	-21.582	3.555	1.00	17.96
3537	C	LEU	B	965	-37.26	-21.744	3.355	1.00	17.73
3538	O	LEU	B	965	-36.814	-22.305	2.362	1.00	19.91
3539	CB	LEU	B	965	-39.468	-22.933	3.402	1.00	17.49
3540	CG	LEU	B	965	-39.647	-23.834	4.626	1.00	20.04
3541	CD1	LEU	B	965	-40.232	-23.041	5.803	1.00	18.62
3542	CD2	LEU	B	965	-40.575	-24.987	4.245	1.00	19.03
3543	N	ALA	B	966	-36.485	-21.235	4.304	1.00	17.16
3544	CA	ALA	B	966	-35.026	-21.304	4.26	1.00	15
3545	C	ALA	B	966	-34.554	-21.183	5.697	1.00	14.76
3546	O	ALA	B	966	-35.322	-20.741	6.559	1.00	14.21
3547	CB	ALA	B	966	-34.461	-20.146	3.43	1.00	15.88
3548	N	ALA	B	967	-33.303	-21.557	5.95	1.00	11.59
3549	CA	ALA	B	967	-32.74	-21.49	7.294	1.00	11.35
3550	C	ALA	B	967	-32.827	-20.097	7.92	1.00	11.98
3551	O	ALA	B	967	-32.945	-19.971	9.138	1.00	14.05
3552	CB	ALA	B	967	-31.286	-21.954	7.276	1.00	11.08
3553	N	ARG	B	968	-32.756	-19.053	7.101	1.00	10.89
3554	CA	ARG	B	968	-32.83	-17.697	7.626	1.00	12.44
3555	C	ARG	B	968	-34.206	-17.383	8.21	1.00	11.97
3556	O	ARG	B	968	-34.341	-16.437	8.987	1.00	11.62
3557	CB	ARG	B	968	-32.498	-16.676	6.533	1.00	12.49
3558	CG	ARG	B	968	-33.396	-16.776	5.331	1.00	13.07
3559	CD	ARG	B	968	-33.088	-15.705	4.3	1.00	13.79

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

3560	NE	ARG	B	968	-33.903	-15.928	3.115	1.00	16.1
3561	CZ	ARG	B	968	-33.593	-16.778	2.144	1.00	16.93
3562	NH1	ARG	B	968	-32.468	-17.48	2.208	1.00	19.1
3563	NH2	ARG	B	968	-34.426	-16.957	1.129	1.00	16.58
3564	N	ASN	B	969	-35.216	-18.171	7.831	1.00	10.71
3565	CA	ASN	B	969	-36.583	-17.981	8.318	1.00	9.71
3566	C	ASN	B	969	-36.995	-19.015	9.373	1.00	10.11
3567	O	ASN	B	969	-38.188	-19.25	9.623	1.00	7.45
3568	CB	ASN	B	969	-37.587	-18.004	7.154	1.00	8.22
3569	CG	ASN	B	969	-37.505	-16.756	6.28	1.00	9.83
3570	OD1	ASN	B	969	-37.359	-15.639	6.777	1.00	8.27
3571	ND2	ASN	B	969	-37.611	-16.946	4.97	1.00	9.41
3572	N	ILE	B	970	-35.999	-19.656	9.97	1.00	9.11
3573	CA	ILE	B	970	-36.259	-20.617	11.025	1.00	9.64
3574	C	ILE	B	970	-35.622	-20.006	12.273	1.00	10.83
3575	O	ILE	B	970	-34.509	-19.461	12.227	1.00	8.79
3576	CB	ILE	B	970	-35.605	-21.995	10.746	1.00	11.81
3577	CG1	ILE	B	970	-36.133	-22.584	9.434	1.00	11.5
3578	CG2	ILE	B	970	-35.872	-22.944	11.913	1.00	7.27
3579	CD1	ILE	B	970	-37.633	-22.852	9.413	1.00	10.46
3580	N	LEU	B	971	-36.327	-20.077	13.389	1.00	10.11
3581	CA	LEU	B	971	-35.775	-19.524	14.605	1.00	12.43
3582	C	LEU	B	971	-35.501	-20.635	15.589	1.00	13.53
3583	O	LEU	B	971	-36.296	-21.565	15.734	1.00	16.02
3584	CB	LEU	B	971	-36.735	-18.471	15.17	1.00	10.99
3585	CG	LEU	B	971	-36.788	-17.337	14.133	1.00	11.75
3586	CD1	LEU	B	971	-38.162	-16.708	14.085	1.00	12.1
3587	CD2	LEU	B	971	-35.679	-16.321	14.44	1.00	6.01
3588	N	VAL	B	972	-34.341	-20.56	16.228	1.00	15.07
3589	CA	VAL	B	972	-33.942	-21.552	17.217	1.00	13.76
3590	C	VAL	B	972	-34.373	-20.99	18.561	1.00	14.71
3591	O	VAL	B	972	-33.759	-20.061	19.088	1.00	13.11
3592	CB	VAL	B	972	-32.42	-21.772	17.189	1.00	12.18
3593	CG1	VAL	B	972	-32.026	-22.83	18.206	1.00	11.65
3594	CG2	VAL	B	972	-31.993	-22.195	15.783	1.00	12.9
3595	N	GLY	B	973	-35.452	-21.55	19.099	1.00	16.73
3596	CA	GLY	B	973	-35.975	-21.072	20.361	1.00	19.14
3597	C	GLY	B	973	-35.476	-21.771	21.603	1.00	21.1
3598	O	GLY	B	973	-34.471	-22.492	21.587	1.00	19.09
3599	N	GLU	B	974	-36.202	-21.534	22.691	1.00	24.39

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## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

3600	CA	GLU	B	974	-35.892	-22.119	23.99	1.00	26.26
3601	C	GLU	B	974	-35.751	-23.634	23.839	1.00	24.81
3602	O	GLU	B	974	-36.476	-24.264	23.066	1.00	23.11
3603	CB	GLU	B	974	-37.013	-21.781	24.98	1.00	29.09
3604	CG	GLU	B	974	-36.752	-22.195	26.424	1.00	35.78
3605	CD	GLU	B	974	-35.663	-21.369	27.1	1.00	38.49
3606	OE1	GLU	B	974	-35.68	-20.126	26.97	1.00	40.76
3607	OE2	GLU	B	974	-34.798	-21.963	27.779	1.00	40.46
3608	N	ASN	B	975	-34.81	-24.204	24.581	1.00	24.95
3609	CA	ASN	B	975	-34.541	-25.639	24.545	1.00	25.27
3610	C	ASN	B	975	-34.093	-26.073	23.15	1.00	22.68
3611	O	ASN	B	975	-34.058	-27.258	22.826	1.00	21.93
3612	CB	ASN	B	975	-35.778	-26.429	24.987	1.00	27.49
3613	CG	ASN	B	975	-35.49	-27.912	25.156	1.00	31.15
3614	OD1	ASN	B	975	-34.384	-28.303	25.553	1.00	31.43
3615	ND2	ASN	B	975	-36.485	-28.748	24.865	1.00	33.71
3616	N	TYR	B	976	-33.744	-25.09	22.331	1.00	21.73
3617	CA	TYR	B	976	-33.273	-25.336	20.975	1.00	20.72
3618	C	TYR	B	976	-34.321	-25.954	20.062	1.00	19.32
3619	O	TYR	B	976	-34.009	-26.78	19.21	1.00	21.32
3620	CB	TYR	B	976	-32.008	-26.201	21.003	1.00	20.1
3621	CG	TYR	B	976	-30.872	-25.554	21.772	1.00	23.99
3622	CD1	TYR	B	976	-30.794	-25.647	23.167	1.00	24.8
3623	CD2	TYR	B	976	-29.891	-24.819	21.109	1.00	25.57
3624	CE1	TYR	B	976	-29.762	-25.023	23.876	1.00	25.21
3625	CE2	TYR	B	976	-28.862	-24.193	21.806	1.00	25.84
3626	CZ	TYR	B	976	-28.801	-24.297	23.183	1.00	26.71
3627	OH	TYR	B	976	-27.772	-23.668	23.854	1.00	29.67
3628	N	VAL	B	977	-35.569	-25.544	20.253	1.00	16.49
3629	CA	VAL	B	977	-36.661	-26.014	19.424	1.00	15.93
3630	C	VAL	B	977	-36.724	-25.09	18.199	1.00	15.18
3631	O	VAL	B	977	-36.813	-23.87	18.343	1.00	15.44
3632	CB	VAL	B	977	-38.008	-25.932	20.177	1.00	16.13
3633	CG1	VAL	B	977	-39.168	-26.154	19.21	1.00	14.17
3634	CG2	VAL	B	977	-38.038	-26.96	21.295	1.00	15.32
3635	N	ALA	B	978	-36.665	-25.666	17.001	1.00	11.85
3636	CA	ALA	B	978	-36.732	-24.863	15.784	1.00	11.3
3637	C	ALA	B	978	-38.163	-24.38	15.554	1.00	11.37
3638	O	ALA	B	978	-39.113	-25.153	15.66	1.00	9.7
3639	CB	ALA	B	978	-36.247	-25.673	14.585	1.00	8.43

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

3640	N	LYS	B	979	-38.309	-23.09	15.258	1.00	13.65
3641	CA	LYS	B	979	-39.623	-22.491	15.011	1.00	13.89
3642	C	LYS	B	979	-39.67	-21.748	13.68	1.00	14.63
3643	O	LYS	B	979	-38.79	-20.936	13.369	1.00	15.95
3644	CB	LYS	B	979	-39.98	-21.536	16.143	1.00	12.45
3645	CG	LYS	B	979	-40.303	-22.24	17.443	1.00	14.01
3646	CD	LYS	B	979	-40.428	-21.26	18.596	1.00	15.7
3647	CE	LYS	B	979	-40.803	-21.972	19.885	1.00	17.99
3648	NZ	LYS	B	979	-42.187	-22.502	19.819	1.00	18.41
3649	N	ILE	B	980	-40.703	-22.027	12.897	1.00	12.5
3650	CA	ILE	B	980	-40.866	-21.393	11.598	1.00	11.81
3651	C	ILE	B	980	-41.36	-19.941	11.676	1.00	12.76
3652	O	ILE	B	980	-42.369	-19.653	12.334	1.00	12.91
3653	CB	ILE	B	980	-41.862	-22.187	10.737	1.00	11.15
3654	CG1	ILE	B	980	-41.375	-23.626	10.588	1.00	10.24
3655	CG2	ILE	B	980	-42.032	-21.519	9.373	1.00	7.93
3656	CD1	ILE	B	980	-42.387	-24.545	9.917	1.00	12.91
3657	N	ALA	B	981	-40.651	-19.034	11.003	1.00	13.06
3658	CA	ALA	B	981	-41.048	-17.625	10.964	1.00	13.31
3659	C	ALA	B	981	-42.306	-17.624	10.103	1.00	15.18
3660	O	ALA	B	981	-42.296	-18.099	8.96	1.00	16.37
3661	CB	ALA	B	981	-39.948	-16.772	10.335	1.00	12.14
3662	N	ASP	B	982	-43.387	-17.085	10.653	1.00	16.3
3663	CA	ASP	B	982	-44.674	-17.114	9.981	1.00	17.39
3664	C	ASP	B	982	-45.407	-15.795	9.726	1.00	18.73
3665	O	ASP	B	982	-46.641	-15.753	9.771	1.00	17.81
3666	CB	ASP	B	982	-45.588	-18.067	10.76	1.00	16.85
3667	CG	ASP	B	982	-45.559	-17.799	12.266	1.00	16.11
3668	OD1	ASP	B	982	-46.094	-18.622	13.041	1.00	13.7
3669	OD2	ASP	B	982	-45.001	-16.756	12.673	1.00	16.18
3670	N	PHE	B	983	-44.665	-14.728	9.455	1.00	19.4
3671	CA	PHE	B	983	-45.289	-13.447	9.152	1.00	20.38
3672	C	PHE	B	983	-45.336	-13.297	7.624	1.00	20.62
3673	O	PHE	B	983	-44.381	-13.656	6.932	1.00	19.69
3674	CB	PHE	B	983	-44.478	-12.289	9.741	1.00	20.89
3675	CG	PHE	B	983	-45.111	-10.936	9.523	1.00	19.99
3676	CD1	PHE	B	983	-46.08	-10.455	10.4	1.00	22.12
3677	CD2	PHE	B	983	-44.762	-10.158	8.424	1.00	19.98
3678	CE1	PHE	B	983	-46.699	-9.212	10.188	1.00	22.49
3679	CE2	PHE	B	983	-45.374	-8.912	8.198	1.00	20.33

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

3680	CZ	PHE	B	983	-46.343	-8.441	9.083	1.00	21.38
3681	N	GLY	B	984	-46.445	-12.777	7.105	1.00	21.49
3682	CA	GLY	B	984	-46.574	-12.575	5.67	1.00	20.35
3683	C	GLY	B	984	-46.81	-13.825	4.837	1.00	21.28
3684	O	GLY	B	984	-46.532	-13.833	3.636	1.00	22.6
3685	N	LEU	B	985	-47.334	-14.879	5.453	1.00	19.77
3686	CA	LEU	B	985	-47.575	-16.117	4.723	1.00	19.13
3687	C	LEU	B	985	-48.868	-16.082	3.912	1.00	19
3688	O	LEU	B	985	-49.748	-15.25	4.154	1.00	18.9
3689	CB	LEU	B	985	-47.619	-17.309	5.688	1.00	17.64
3690	CG	LEU	B	985	-46.464	-17.483	6.68	1.00	15.46
3691	CD1	LEU	B	985	-46.542	-18.886	7.253	1.00	12.99
3692	CD2	LEU	B	985	-45.117	-17.264	6.001	1.00	14.4
3693	N	SER	B	986	-48.968	-16.991	2.947	1.00	18.22
3694	CA	SER	B	986	-50.151	-17.103	2.102	1.00	18.43
3695	C	SER	B	986	-51.018	-18.257	2.592	1.00	19.51
3696	O	SER	B	986	-50.574	-19.119	3.363	1.00	16.3
3697	CB	SER	B	986	-49.766	-17.357	0.642	1.00	18.37
3698	OG	SER	B	986	-49.049	-16.259	0.102	1.00	20.94
3699	N	ARG	B	987	-52.255	-18.279	2.117	1.00	20.32
3700	CA	ARG	B	987	-53.181	-19.309	2.519	1.00	20.23
3701	C	ARG	B	987	-54.086	-19.617	1.345	1.00	19.36
3702	O	ARG	B	987	-54.641	-18.711	0.743	1.00	20.5
3703	CB	ARG	B	987	-53.978	-18.801	3.711	1.00	21.67
3704	CG	ARG	B	987	-54.676	-19.871	4.494	1.00	26.66
3705	CD	ARG	B	987	-54.676	-19.524	5.971	1.00	28.38
3706	NE	ARG	B	987	-55.412	-20.523	6.735	1.00	30.66
3707	CZ	ARG	B	987	-56.728	-20.661	6.693	1.00	30.77
3708	NH1	ARG	B	987	-57.449	-19.857	5.926	1.00	33.61
3709	NH2	ARG	B	987	-57.323	-21.605	7.407	1.00	33.56
3710	N	GLY	B	988	-54.221	-20.899	1.019	1.00	20.04
3711	CA	GLY	B	988	-55.058	-21.305	-0.099	1.00	19.9
3712	C	GLY	B	988	-54.427	-22.46	-0.864	1.00	22.02
3713	O	GLY	B	988	-53.519	-23.113	-0.35	1.00	22.37
3714	N	GLN	B	989	-54.905	-22.703	-2.084	1.00	21.84
3715	CA	GLN	B	989	-54.407	-23.776	-2.946	1.00	23.31
3716	C	GLN	B	989	-53.09	-23.428	-3.614	1.00	23.16
3717	O	GLN	B	989	-52.177	-24.252	-3.692	1.00	21.35
3718	CB	GLN	B	989	-55.405	-24.073	-4.071	1.00	26.7
3719	CG	GLN	B	989	-56.644	-24.816	-3.657	1.00	31.75



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TABLE 3

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

3720	CD	GLN	B	989	-56.325	-26.202	-3.171	1.00	32.68
3721	OE1	GLN	B	989	-55.772	-27.014	-3.912	1.00	33.69
3722	NE2	GLN	B	989	-56.664	-26.484	-1.917	1.00	34.03
3723	N	GLU	B	990	-53.028	-22.204	-4.127	1.00	23.44
3724	CA	GLU	B	990	-51.866	-21.713	-4.852	1.00	24.74
3725	C	GLU	B	990	-51.87	-20.192	-4.784	1.00	21.97
3726	O	GLU	B	990	-52.916	-19.582	-4.591	1.00	21.65
3727	CB	GLU	B	990	-51.965	-22.175	-6.314	1.00	27.17
3728	CG	GLU	B	990	-50.841	-21.74	-7.238	1.00	35.77
3729	CD	GLU	B	990	-51.038	-22.249	-8.663	1.00	39.4
3730	OE1	GLU	B	990	-51.242	-23.463	-8.837	1.00	35.11
3731	OE2	GLU	B	990	-50.987	-21.441	-9.611	1.00	44.6
3732	N	VAL	B	991	-50.698	-19.586	-4.928	1.00	19.64
3733	CA	VAL	B	991	-50.595	-18.138	-4.906	1.00	19.2
3734	C	VAL	B	991	-49.601	-17.663	-5.959	1.00	19.72
3735	O	VAL	B	991	-48.526	-18.242	-6.127	1.00	20.52
3736	CB	VAL	B	991	-50.159	-17.603	-3.504	1.00	18.83
3737	CG1	VAL	B	991	-48.877	-18.287	-3.038	1.00	17.66
3738	CG2	VAL	B	991	-49.941	-16.11	-3.575	1.00	18.19
3739	N	TYR	B	992	-49.979	-16.621	-6.687	1.00	20.76
3740	CA	TYR	B	992	-49.112	-16.046	-7.704	1.00	21.59
3741	C	TYR	B	992	-48.535	-14.757	-7.131	1.00	22.71
3742	O	TYR	B	992	-49.28	-13.899	-6.666	1.00	24.45
3743	CB	TYR	B	992	-49.901	-15.727	-8.977	1.00	21.07
3744	CG	TYR	B	992	-49.172	-14.781	-9.907	1.00	22.61
3745	CD1	TYR	B	992	-48.202	-15.244	-10.798	1.00	22
3746	CD2	TYR	B	992	-49.404	-13.406	-9.845	1.00	22.89
3747	CE1	TYR	B	992	-47.483	-14.36	-11.598	1.00	23.24
3748	CE2	TYR	B	992	-48.691	-12.517	-10.632	1.00	23.56
3749	CZ	TYR	B	992	-47.734	-12.993	-11.506	1.00	24.84
3750	OH	TYR	B	992	-47.036	-12.096	-12.287	1.00	27.04
3751	N	VAL	B	993	-47.214	-14.628	-7.151	1.00	24.51
3752	CA	VAL	B	993	-48.556	-13.427	-6.643	1.00	27.37
3753	C	VAL	B	993	-45.546	-12.957	-7.681	1.00	29.51
3754	O	VAL	B	993	-44.59	-13.666	-7.99	1.00	30.36
3755	CB	VAL	B	993	-45.816	-13.702	-5.317	1.00	27.6
3756	CG1	VAL	B	993	-45.23	-12.407	-4.773	1.00	26.53
3757	CG2	VAL	B	993	-46.769	-14.324	-4.305	1.00	26.44
3758	N	ALA	B	994	-45.769	-11.771	-8.237	1.00	32.75
3759	CA	ALA	B	994	-44.868	-11.23	-9.25	1.00	36.29

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TABLE 3

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

3760	C	ALA	B	994	-43.559	-10.797	-8.608	1.00	38.02
3761	O	ALA	B	994	-43.542	-10.369	-7.455	1.00	38.12
3762	CB	ALA	B	994	-45.522	-10.04	-9.959	1.00	36.41
3763	N	ALA	B	995	-42.466	-10.91	-9.355	1.00	41.47
3764	CA	ALA	B	995	-41.152	-10.517	-8.849	1.00	45.29
3765	CB	ALA	B	995	-40.093	-10.718	-9.931	1.00	44.84
3766	C	ALA	B	995	-41.162	-9.054	-8.388	1.00	47.22
3767	OT1	ALA	B	995	-40.89	-8.804	-7.191	1.00	48.44
3768	OT2	ALA	B	995	-41.446	-8.172	-9.23	1.00	48.79
3769	N	LEU	B	0	-31.418	-13.078	-1.057	1.00	46.59
3770	CA	LEU	B	0	-31.7	-13.774	-2.344	1.00	45.62
3771	C	LEU	B	0	-32.824	-14.794	-2.157	1.00	45.78
3772	O	LEU	B	0	-32.942	-15.407	-1.095	1.00	47.94
3773	CB	LEU	B	0	-30.431	-14.469	-2.846	1.00	45.19
3774	CG	LEU	B	0	-30.547	-15.308	-4.12	1.00	44.58
3775	CD1	LEU	B	0	-29.164	-15.501	-4.748	1.00	45.23
3776	CD2	LEU	B	0	-31.199	-16.642	-3.783	1.00	41.08
3777	N	PRO	B	1	-33.668	-14.986	-3.188	1.00	44.07
3778	CA	PRO	B	1	-34.776	-15.946	-3.086	1.00	40.46
3779	C	PRO	B	1	-34.692	-17.15	-4.039	1.00	36.49
3780	O	PRO	B	1	-35.099	-18.261	-3.701	1.00	34.87
3781	CB	PRO	B	1	-35.976	-15.071	-3.396	1.00	41.04
3782	CG	PRO	B	1	-35.433	-14.212	-4.56	1.00	42.22
3783	CD	PRO	B	1	-33.945	-13.983	-4.24	1.00	42.84
3784	N	VAL	B	2	-34.166	-16.908	-5.231	1.00	32.85
3785	CA	VAL	B	2	-34.053	-17.92	-6.274	1.00	29.48
3786	C	VAL	B	2	-33.431	-19.273	-5.916	1.00	26.72
3787	O	VAL	B	2	-33.916	-20.308	-6.372	1.00	23.74
3788	CB	VAL	B	2	-33.304	-17.325	-7.502	1.00	29.84
3789	CG1	VAL	B	2	-32.036	-16.668	-7.049	1.00	31.31
3790	CG2	VAL	B	2	-32.984	-18.408	-8.519	1.00	29.98
3791	N	ARG	B	3	-32.375	-19.274	-5.105	1.00	24.35
3792	CA	ARG	B	3	-31.634	-20.516	-4.743	1.00	22.17
3793	C	ARG	B	3	-32.524	-21.532	-3.96	1.00	19.83
3794	O	ARG	B	3	-32.11	-22.677	-3.796	1.00	17.92
3795	CB	ARG	B	3	-30.396	-20.18	-3.978	1.00	24.31
3796	CG	ARG	B	3	-29.578	-19.08	-4.667	1.00	27.02
3797	CD	ARG	B	3	-28.412	-18.576	-3.826	1.00	27.98
3798	NE	ARG	B	3	-27.166	-19.192	-4.257	1.00	32.91
3799	CZ	ARG	B	3	-26.444	-18.794	-5.301	1.00	32.28

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TABLE 3

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

3800	NH1	ARG	B	3	-26.824	-17.755	-6.033	1.00	33.47
3801	NH2	ARG	B	3	-25.356	-19.469	-5.636	1.00	33.28
3802	N	TRP	B	4	-33.695	-21.112	-3.482	1.00	16.47
3803	CA	TRP	B	4	-34.59	-21.991	-2.736	1.00	15.08
3804	C	TRP	B	4	-35.903	-22.204	-3.483	1.00	15.56
3805	O	TRP	B	4	-36.793	-22.907	-2.999	1.00	16.61
3806	CB	TRP	B	4	-34.943	-21.387	-1.377	1.00	13.74
3807	CG	TRP	B	4	-33.89	-21.459	-0.329	1.00	13.42
3808	CD1	TRP	B	4	-33.872	-22.291	0.761	1.00	11.29
3809	CD2	TRP	B	4	-32.718	-20.643	-0.233	1.00	12.62
3810	NE1	TRP	B	4	-32.764	-22.04	1.527	1.00	10.8
3811	CE2	TRP	B	4	-32.034	-21.034	0.943	1.00	12.27
3812	CE3	TRP	B	4	-32.177	-19.617	-1.026	1.00	14.19
3813	CZ2	TRP	B	4	-30.828	-20.435	1.349	1.00	11.75
3814	CZ3	TRP	B	4	-30.969	-19.014	-0.619	1.00	13.56
3815	CH2	TRP	B	4	-30.313	-19.431	0.56	1.00	13.35
3816	N	MET	B	5	-36.047	-21.587	-4.645	1.00	14.4
3817	CA	MET	B	5	-37.296	-21.72	-5.385	1.00	16.61
3818	C	MET	B	5	-37.407	-22.965	-6.248	1.00	16.62
3819	O	MET	B	5	-36.431	-23.428	-6.829	1.00	15.42
3820	CB	MET	B	5	-37.532	-20.479	-6.256	1.00	17.73
3821	CG	MET	B	5	-37.996	-19.26	-5.476	1.00	19.13
3822	SD	MET	B	5	-37.722	-17.723	-6.37	1.00	21.97
3823	CE	MET	B	5	-38.872	-17.905	-7.767	1.00	17.11
3824	N	ALA	B	6	-38.616	-23.51	-6.314	1.00	17.72
3825	CA	ALA	B	6	-38.873	-24.684	-7.139	1.00	19.53
3826	C	ALA	B	6	-38.881	-24.213	-8.597	1.00	19.44
3827	O	ALA	B	6	-39.063	-23.024	-8.873	1.00	19.75
3828	CB	ALA	B	6	-40.229	-25.301	-6.766	1.00	18.45
3829	N	ILE	B	7	-38.682	-25.136	-9.527	1.00	19.52
3830	CA	ILE	B	7	-38.675	-24.783	-10.939	1.00	20.91
3831	C	ILE	B	7	-39.945	-24.034	-11.341	1.00	20.57
3832	O	ILE	B	7	-39.875	-22.999	-12.006	1.00	20.25
3833	CB	ILE	B	7	-38.555	-26.034	-11.83	1.00	22.59
3834	CG1	ILE	B	7	-37.269	-26.794	-11.497	1.00	23.2
3835	CG2	ILE	B	7	-38.562	-25.623	-13.296	1.00	23.26
3836	CD1	ILE	B	7	-37.124	-28.116	-12.245	1.00	23.3
3837	N	GLU	B	8	-41.102	-24.555	-10.934	1.00	19.67
3838	CA	GLU	B	8	-42.367	-23.921	-11.285	1.00	19.63
3839	C	GLU	B	8	-42.471	-22.503	-10.731	1.00	19.13

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

3840	O	GLU	B	8	-43.154	-21.653	-11.302	1.00	19.29
3841	CB	GLU	B	8	-43.554	-24.76	-10.799	1.00	18.42
3842	CG	GLU	B	8	-43.693	-24.817	-9.294	1.00	21.17
3843	CD	GLU	B	8	-43.23	-26.133	-8.703	1.00	20.65
3844	OE1	GLU	B	8	-42.169	-26.65	-9.128	1.00	19.6
3845	OE2	GLU	B	8	-43.929	-26.639	-7.802	1.00	20.25
3846	N	SER	B	9	-41.801	-22.238	-9.618	1.00	18.54
3847	CA	SER	B	9	-41.849	-20.892	-9.061	1.00	19.66
3848	C	SER	B	9	-40.948	-19.995	-9.892	1.00	19.48
3849	O	SER	B	9	-41.314	-18.874	-10.229	1.00	20.15
3850	CB	SER	B	9	-41.398	-20.883	-7.596	1.00	19.67
3851	OG	SER	B	9	-42.331	-21.572	-6.773	1.00	20.35
3852	N	LEU	B	10	-39.766	-20.496	-10.231	1.00	19.94
3853	CA	LEU	B	10	-38.831	-19.723	-11.034	1.00	20.3
3854	C	LEU	B	10	-39.481	-19.375	-12.367	1.00	20.91
3855	O	LEU	B	10	-39.367	-18.244	-12.832	1.00	21.91
3856	CB	LEU	B	10	-37.544	-20.519	-11.28	1.00	18.05
3857	CG	LEU	B	10	-36.638	-20.805	-10.079	1.00	16.79
3858	CD1	LEU	B	10	-35.653	-21.915	-10.444	1.00	15.16
3859	CD2	LEU	B	10	-35.897	-19.533	-9.663	1.00	13.45
3860	N	ASN	B	11	-40.172	-20.344	-12.965	1.00	20.77
3861	CA	ASN	B	11	-40.834	-20.14	-14.255	1.00	22.52
3862	C	ASN	B	11	-42.075	-19.249	-14.281	1.00	22.85
3863	O	ASN	B	11	-42.159	-18.342	-15.101	1.00	23.83
3864	CB	ASN	B	11	-41.223	-21.481	-14.888	1.00	22.83
3865	CG	ASN	B	11	-40.022	-22.289	-15.332	1.00	24.69
3866	OD1	ASN	B	11	-38.944	-21.74	-15.563	1.00	25.31
3867	ND2	ASN	B	11	-40.206	-23.601	-15.473	1.00	22.9
3868	N	TYR	B	12	-43.039	-19.505	-13.397	1.00	23.13
3869	CA	TYR	B	12	-44.278	-18.734	-13.405	1.00	22.43
3870	C	TYR	B	12	-44.624	-17.962	-12.144	1.00	22.05
3871	O	TYR	B	12	-45.727	-17.433	-12.024	1.00	21.46
3872	CB	TYR	B	12	-45.447	-19.654	-13.747	1.00	23.93
3873	CG	TYR	B	12	-45.178	-20.566	-14.918	1.00	27.33
3874	CD1	TYR	B	12	-44.928	-21.928	-14.723	1.00	27.44
3875	CD2	TYR	B	12	-45.168	-20.07	-16.229	1.00	27.52
3876	CE1	TYR	B	12	-44.676	-22.779	-15.807	1.00	30.15
3877	CE2	TYR	B	12	-44.917	-20.91	-17.319	1.00	28.84
3878	CZ	TYR	B	12	-44.674	-22.264	-17.101	1.00	30.87
3879	OH	TYR	B	12	-44.441	-23.104	-18.173	1.00	33.82

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

3880	N	SER	B	13	-43.698	-17.896	-11.2	1.00	22.05
3881	CA	SER	B	13	-43.949	-17.171	-9.962	1.00	22.52
3882	C	SER	B	13	-45.142	-17.719	-9.178	1.00	21.71
3883	O	SER	B	13	-45.861	-16.968	-8.515	1.00	20.78
3884	CB	SER	B	13	-44.165	-15.683	-10.265	1.00	24.13
3885	OG	SER	B	13	-43.053	-15.147	-10.975	1.00	27.56
3886	N	VAL	B	14	-45.357	-19.027	-9.255	1.00	20.94
3887	CA	VAL	B	14	-46.45	-19.645	-8.516	1.00	22.09
3888	C	VAL	B	14	-45.897	-20.371	-7.291	1.00	21.8
3889	O	VAL	B	14	-44.769	-20.857	-7.313	1.00	22.49
3890	CB	VAL	B	14	-47.236	-20.658	-9.39	1.00	23.23
3891	CG1	VAL	B	14	-48.093	-19.919	-10.402	1.00	21.44
3892	CG2	VAL	B	14	-46.268	-21.6	-10.101	1.00	24.54
3893	N	TYR	B	15	-46.679	-20.417	-6.217	1.00	21.15
3894	CA	TYR	B	15	-46.263	-21.105	-4.993	1.00	19.73
3895	C	TYR	B	15	-47.374	-22.017	-4.459	1.00	18.83
3896	O	TYR	B	15	-48.556	-21.644	-4.444	1.00	16.53
3897	CB	TYR	B	15	-45.858	-20.093	-3.91	1.00	20.44
3898	CG	TYR	B	15	-44.752	-19.159	-4.337	1.00	22.2
3899	CD1	TYR	B	15	-45.032	-10.023	-5.096	1.00	22.86
3900	CD2	TYR	B	15	-43.411	-19.452	-4.054	1.00	21.94
3901	CE1	TYR	B	15	-44.008	-17.206	-5.572	1.00	23.92
3902	CE2	TYR	B	15	-42.379	-18.638	-4.526	1.00	21.57
3903	CZ	TYR	B	15	-42.685	-17.52	-5.288	1.00	22.46
3904	OH	TYR	B	15	-41.678	-16.73	-5.795	1.00	22.84
3905	N	THR	B	16	-46.972	-23.209	-4.026	1.00	17.99
3906	CA	THR	B	16	-47.875	-24.223	-3.473	1.00	18.44
3907	C	THR	B	16	-47.134	-24.899	-2.316	1.00	20.08
3908	O	THR	B	16	-45.953	-24.619	-2.088	1.00	19.39
3909	CB	THR	B	16	-48.216	-25.317	-4.517	1.00	18.02
3910	OG1	THR	B	16	-47.031	-26.069	-4.824	1.00	18.21
3911	CG2	THR	B	16	-48.759	-24.696	-5.801	1.00	15.39
3912	N	THR	B	17	-47.81	-25.781	-1.582	1.00	20.61
3913	CA	THR	B	17	-47.139	-26.473	-0.489	1.00	20.94
3914	C	THR	B	17	-46.125	-27.408	-1.145	1.00	20.16
3915	O	THR	B	17	-45.104	-27.766	-0.545	1.00	20.22
3916	CB	THR	B	17	-48.113	-27.304	0.377	1.00	21.34
3917	OG1	THR	B	17	-48.626	-28.392	-0.395	1.00	23.5
3918	CG2	THR	B	17	-49.272	-26.442	0.86	1.00	21.93
3919	N	ASN	B	18	-46.403	-27.793	-2.388	1.00	19.73

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

3920	CA	ASN	B	18	-45.486	-28.664	-3.113	1.00	19.9
3921	C	ASN	B	18	-44.156	-27.95	-3.308	1.00	18.53
3922	O	ASN	B	18	-43.1	-28.567	-3.207	1.00	19.74
3923	CB	ASN	B	18	-46.065	-29.077	-4.47	1.00	22.04
3924	CG	ASN	B	18	-47.008	-30.269	-4.364	1.00	24.22
3925	OD1	ASN	B	18	-46.761	-31.201	-3.598	1.00	24.23
3926	ND2	ASN	B	18	-48.082	-30.253	-5.149	1.00	24.37
3927	N	SER	B	19	-44.201	-26.647	-3.574	1.00	16.65
3928	CA	SER	B	19	-42.969	-25.896	-3.754	1.00	14.69
3929	C	SER	B	19	-42.314	-25.561	-2.411	1.00	14.96
3930	O	SER	B	19	-41.107	-25.322	-2.356	1.00	15.63
3931	CB	SER	B	19	-43.21	-24.629	-4.594	1.00	14.1
3932	OG	SER	B	19	-44.33	-23.874	-4.16	1.00	13.54
3933	N	ASP	B	20	-43.09	-25.543	-1.326	1.00	13.38
3934	CA	ASP	B	20	-42.498	-25.281	-0.012	1.00	13.53
3935	C	ASP	B	20	-41.603	-26.484	0.294	1.00	13.78
3936	O	ASP	B	20	-40.525	-26.346	0.89	1.00	14.34
3937	CB	ASP	B	20	-43.561	-25.162	1.091	1.00	12.01
3938	CG	ASP	B	20	-44.154	-23.771	1.191	1.00	13.56
3939	OD1	ASP	B	20	-43.48	-22.793	0.788	1.00	14.11
3940	OD2	ASP	B	20	-45.295	-23.658	1.691	1.00	12.37
3941	N	VAL	B	21	-42.068	-27.66	-0.12	1.00	10.87
3942	CA	VAL	B	21	-41.333	-28.902	0.073	1.00	11.68
3943	C	VAL	B	21	-39.971	-28.812	-0.625	1.00	13.21
3944	O	VAL	B	21	-38.952	-29.277	-0.092	1.00	13.17
3945	CB	VAL	B	21	-42.145	-30.099	-0.483	1.00	11.13
3946	CG1	VAL	B	21	-41.262	-31.335	-0.625	1.00	10.94
3947	CG2	VAL	B	21	-43.324	-30.38	0.446	1.00	9.83
3948	N	TRP	B	22	-39.961	-28.21	-1.815	1.00	13.07
3949	CA	TRP	B	22	-38.729	-28.028	-2.575	1.00	13.39
3950	C	TRP	B	22	-37.799	-27.156	-1.74	1.00	13.64
3951	O	TRP	B	22	-36.618	-27.461	-1.571	1.00	14.75
3952	CB	TRP	B	22	39.03	-27.342	-3.908	1.00	14.72
3953	CG	TRP	B	22	-37.813	-27.049	-4.727	1.00	17.45
3954	CD1	TRP	B	22	-36.81	-26.169	-4.426	1.00	16.77
3955	CD2	TRP	B	22	-37.463	-27.642	-5.984	1.00	17.73
3956	NE1	TRP	B	22	-35.86	-26.178	-5.414	1.00	19.32
3957	CE2	TRP	B	22	-36.234	-27.072	-6.384	1.00	19.88
3958	CE3	TRP	B	22	-38.068	-28.598	-6.81	1.00	16.5
3959	CZ2	TRP	B	22	-35.595	-27.427	-7.582	1.00	20.3

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TABLE 3

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

3960	CZ3	TRP	B	22	-37.436	-28.952	-7.998	1.00	18.37
3961	CH2	TRP	B	22	-36.209	-28.365	-8.373	1.00	19.78
3962	N	SER	B	23	-38.335	-26.061	-1.219	1.00	13.41
3963	CA	SER	B	23	-37.544	-25.177	-0.381	1.00	13.86
3964	C	SER	B	23	-37.089	-25.948	0.855	1.00	12.94
3965	O	SER	B	23	-35.978	-25.744	1.34	1.00	13.26
3966	CB	SER	B	23	-38.361	-23.952	0.024	1.00	13.65
3967	OG	SER	B	23	-38.736	-23.217	-1.13	1.00	19.12
3968	N	TYR	B	24	-37.937	-26.838	1.361	1.00	11.03
3969	CA	TYR	B	24	-37.55	-27.63	2.52	1.00	12.19
3970	C	TYR	B	24	-36.304	-28.464	2.166	1.00	11.8
3971	O	TYR	B	24	-35.39	-28.613	2.984	1.00	10.75
3972	CB	TYR	B	24	-38.683	-28.573	2.953	1.00	12
3973	CG	TYR	B	24	-38.271	-29.431	4.117	1.00	12.56
3974	CD1	TYR	B	24	-38.357	-28.952	5.431	1.00	13.29
3975	CD2	TYR	B	24	-37.681	-30.677	3.906	1.00	13.29
3976	CE1	TYR	B	24	-37.859	-29.693	6.497	1.00	11.48
3977	CE2	TYR	B	24	-37.179	-31.427	4.966	1.00	12.38
3978	CZ	TYR	B	24	-37.269	-30.929	6.254	1.00	12.69
3979	OH	TYR	B	24	-36.759	-31.673	7.292	1.00	15.15
3980	N	GLY	B	25	-36.285	-29.008	0.947	1.00	10.56
3981	CA	GLY	B	25	-35.159	-29.813	0.5	1.00	10.28
3982	C	GLY	B	25	-33.854	-29.048	0.607	1.00	11.72
3983	O	GLY	B	25	-32.831	-29.579	1.056	1.00	12.42
3984	N	VAL	B	26	-33.893	-27.79	0.18	1.00	10.92
3985	CA	VAL	B	26	-32.736	-26.917	0.241	1.00	8.29
3986	C	VAL	B	26	-32.437	-26.571	1.717	1.00	8.4
3987	O	VAL	B	26	-31.277	-26.484	2.121	1.00	6.76
3988	CB	VAL	B	26	-33.007	-25.629	-0.569	1.00	8.98
3989	CG1	VAL	B	26	-31.755	-24.746	-0.611	1.00	3.49
3990	CG2	VAL	B	26	-33.467	-26.003	-1.976	1.00	6.14
3991	N	LEU	B	27	-33.479	-26.372	2.52	1.00	8.14
3992	CA	LEU	B	27	-33.284	-26.061	3.933	1.00	8.75
3993	C	LEU	B	27	-32.513	-27.217	4.589	1.00	8.72
3994	O	LEU	B	27	-31.541	-27.005	5.313	1.00	7
3995	CB	LEU	B	27	-34.634	-25.855	4.627	1.00	8.89
3996	CG	LEU	B	27	-34.654	-25.955	6.165	1.00	13.53
3997	CD1	LEU	B	27	-33.642	-24.989	6.795	1.00	14.01
3998	CD2	LEU	B	27	-36.046	-25.628	6.657	1.00	13.01
3999	N	LEU	B	28	-32.95	-28.439	4.314	1.00	8.87

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## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

4000	CA	LEU	B	28	-32.3	-29.626	4.853	1.00	9.56
4001	C	LEU	B	28	-30.844	-29.671	4.401	1.00	10.42
4002	O	LEU	B	28	-29.967	-30.122	5.143	1.00	10.85
4003	CB	LEU	B	28	-33.028	-30.886	4.376	1.00	8.34
4004	CG	LEU	B	28	-32.351	-32.228	4.668	1.00	9.96
4005	CD1	LEU	B	28	-32.223	-32.462	6.172	1.00	10.29
4006	CD2	LEU	B	28	-33.173	-33.33	4.036	1.00	11.57
4007	N	TRP	B	29	-30.595	-29.217	3.173	1.00	11.88
4008	CA	TRP	B	29	-29.242	-29.192	2.615	1.00	11.61
4009	C	TRP	B	29	-28.399	-28.178	3.4	1.00	11.3
4010	O	TRP	B	29	-27.214	-28.405	3.642	1.00	12.24
4011	CB	TRP	B	29	-29.294	-28.805	1.134	1.00	11.64
4012	CG	TRP	B	29	-27.988	-28.924	0.407	1.00	13.59
4013	CD1	TRP	B	29	-27.553	-29.989	-0.335	1.00	13.96
4014	CD2	TRP	B	29	-26.955	-27.928	0.323	1.00	12.22
4015	NE1	TRP	B	29	-26.322	-29.715	-0.879	1.00	13.46
4016	CE2	TRP	B	29	-25.931	-28.458	-0.495	1.00	12.4
4017	CE3	TRP	B	29	-26.799	-26.64	0.857	1.00	10.75
4018	CZ2	TRP	B	29	-24.765	-27.744	-0.796	1.00	11.68
4019	CZ3	TRP	B	29	-25.643	-25.93	0.56	1.00	13.4
4020	CH2	TRP	B	29	-24.636	-26.486	-0.264	1.00	12.64
4021	N	GLU	B	30	-29.014	-27.061	3.792	1.00	12.2
4022	CA	GLU	B	30	-28.324	-26.031	4.575	1.00	12.93
4023	C	GLU	B	30	-27.954	-26.598	5.948	1.00	12.49
4024	O	GLU	B	30	-26.885	-26.306	6.491	1.00	12.85
4025	CB	GLU	B	30	-29.223	-24.807	4.804	1.00	13.8
4026	CG	GLU	B	30	-29.657	-24.024	3.569	1.00	13.8
4027	CD	GLU	B	30	-30.469	-22.791	3.947	1.00	14.49
4028	OE1	GLU	B	30	-29.856	-21.758	4.298	1.00	15.24
4029	OE2	GLU	B	30	-31.719	-22.86	3.92	1.00	13.16
4030	N	ILE	B	31	-28.858	-27.39	6.517	1.00	11.17
4031	CA	ILE	B	31	-28.634	-27.993	7.826	1.00	10.77
4032	C	ILE	B	31	-27.461	-28.961	7.781	1.00	11.23
4033	O	ILE	B	31	-26.55	-28.901	8.608	1.00	10.9
4034	CB	ILE	B	31	-29.882	-28.767	8.31	1.00	10.5
4035	CG1	ILE	B	31	-31.06	-27.802	8.505	1.00	9.63
4036	CG2	ILE	B	31	-29.559	-29.501	9.602	1.00	9.48
4037	CD1	ILE	B	31	-32.266	-28.445	9.178	1.00	8.92
4038	N	VAL	B	32	-27.502	-29.853	6.801	1.00	11.75
4039	CA	VAL	B	32	-26.47	-30.86	6.61	1.00	11.98



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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

4040	C	VAL	B	32	-25.117	-30.203	6.335	1.00	13.66
4041	O	VAL	B	32	-24.095	-30.623	6.885	1.00	12.57
4042	CB	VAL	B	32	-26.87	-31.808	5.434	1.00	11.36
4043	CG1	VAL	B	32	-25.753	-32.786	5.118	1.00	9.08
4044	CG2	VAL	B	32	-28.143	-32.567	5.807	1.00	10.62
4045	N	SER	B	33	-25.117	-29.162	5.503	1.00	14.52
4046	CA	SER	B	33	-23.881	-28.465	5.147	1.00	15.93
4047	C	SER	B	33	-23.455	-27.422	6.165	1.00	16.46
4048	O	SER	B	33	-22.572	-26.611	5.886	1.00	17.58
4049	CB	SER	B	33	-24.016	-27.793	3.781	1.00	16.54
4050	OG	SER	B	33	-24.992	-26.768	3.816	1.00	21.73
4051	N	LEU	B	34	-24.087	-27.447	7.338	1.00	16.38
4052	CA	LEU	B	34	-23.782	-26.522	8.427	1.00	15.03
4053	C	LEU	B	34	-23.86	-25.055	8.02	1.00	16.03
4054	O	LEU	B	34	-22.991	-24.248	8.371	1.00	15.24
4055	CB	LEU	B	34	-22.399	-26.833	9.016	1.00	14.9
4056	CG	LEU	B	34	-22.228	-28.219	9.661	1.00	15.37
4057	CD1	LEU	B	34	-20.768	-28.464	10.006	1.00	13.59
4058	CD2	LEU	B	34	-23.09	-28.317	10.913	1.00	14.14
4059	N	GLY	B	35	-24.906	-24.717	7.27	1.00	15.32
4060	CA	GLY	B	35	-25.105	-23.343	6.856	1.00	14.45
4061	C	GLY	B	35	-24.392	-22.899	5.598	1.00	15.73
4062	O	GLY	B	35	-24.129	-21.704	5.422	1.00	16.23
4063	N	GLY	B	36	-24.073	-23.842	4.719	1.00	16.52
4064	CA	GLY	B	36	-23.403	-23.474	3.484	1.00	16.95
4065	C	GLY	B	36	-24.36	-22.797	2.519	1.00	16.43
4066	O	GLY	B	36	-25.57	-22.996	2.596	1.00	15.81
4067	N	THR	B	37	-23.826	-21.982	1.615	1.00	17.83
4068	CA	THR	B	37	-24.657	-21.293	0.625	1.00	16.72
4069	C	THR	B	37	-25.005	-22.265	-0.495	1.00	16.55
4070	O	THR	B	37	-24.121	-22.816	-1.148	1.00	18.02
4071	CB	THR	B	37	-23.928	-20.091	-0.006	1.00	17.12
4072	OG1	THR	B	37	-23.639	-19.118	1.002	1.00	17.25
4073	CG2	THR	B	37	-24.792	-19.45	-1.093	1.00	16.52
4074	N	PRO	B	38	-26.303	-22.487	-0.732	1.00	16.32
4075	CA	PRO	B	38	-26.764	-23.402	-1.784	1.00	15.31
4076	C	PRO	B	38	-26.251	-22.983	-3.169	1.00	15.08
4077	O	PRO	B	38	-26.322	-21.809	-3.521	1.00	11.22
4078	CB	PRO	B	38	-28.288	-23.297	-1.69	1.00	14.49
4079	CG	PRO	B	38	-28.529	-22.844	-0.274	1.00	15.43

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

4080	CD	PRO	B	38	-27.442	-21.842	-0.056	1.00	13.87
4081	N	TYR	B	39	-25.767	-23.953	-3.946	1.00	17.31
4082	CA	TYR	B	39	-25.235	-23.716	-5.291	1.00	20.08
4083	C	TYR	B	39	-24.073	-22.716	-5.231	1.00	23.4
4084	O	TYR	B	39	-23.851	-21.961	-6.179	1.00	24.29
4085	CB	TYR	B	39	-26.324	-23.156	-6.23	1.00	18.19
4086	CG	TYR	B	39	-27.604	-23.962	-6.312	1.00	16.57
4087	CD1	TYR	B	39	-27.677	-25.147	-7.064	1.00	16.91
4088	CD2	TYR	B	39	-28.741	-23.555	-5.619	1.00	13.79
4089	CE1	TYR	B	39	-28.865	-25.907	-7.112	1.00	12.16
4090	CE2	TYR	B	39	-29.917	-24.297	-5.659	1.00	14.18
4091	CZ	TYR	B	39	-29.978	-25.469	-6.402	1.00	13.48
4092	OH	TYR	B	39	-31.154	-26.187	-6.41	1.00	11.14
4093	N	CYS	B	40	-23.338	-22.708	-4.12	1.00	26.51
4094	CA	CYS	B	40	-22.217	-21.784	-3.944	1.00	29.16
4095	C	CYS	B	40	-21.385	-21.658	-5.213	1.00	30.07
4096	O	CYS	B	40	-20.958	-22.657	-5.784	1.00	29.03
4097	CB	CYS	B	40	-21.314	-22.239	-2.791	1.00	31.18
4098	SG	CYS	B	40	-20.143	-20.957	-2.228	1.00	34.44
4099	N	GLY	B	41	-21.165	-20.422	-5.652	1.00	32.17
4100	CA	GLY	B	41	-20.386	-20.199	-6.854	1.00	33.84
4101	C	GLY	B	41	-21.225	-19.929	-8.094	1.00	35.92
4102	O	GLY	B	41	-20.873	-19.067	-8.907	1.00	36.63
4103	N	MET	B	42	-22.332	-20.655	-8.247	1.00	35.4
4104	CA	MET	B	42	-23.21	-20.489	-9.407	1.00	34.44
4105	C	MET	B	42	-24.019	-19.199	-9.367	1.00	34.26
4106	O	MET	B	42	-24.425	-18.747	-8.301	1.00	33.23
4107	CB	MET	B	42	-24.17	-21.669	-9.509	1.00	34.38
4108	CG	MET	B	42	-23.486	-23.014	-9.65	1.00	35.17
4109	SD	MET	B	42	-24.679	-24.354	-9.74	1.00	36.05
4110	CE	MET	B	42	-25.27	-24.17	-11.442	1.00	36.01
4111	N	THR	B	43	-24.251	-18.607	-10.536	1.00	35.39
4112	CA	THR	B	43	-25.032	-17.375	-10.62	1.00	36.27
4113	C	THR	B	43	-26.509	-17.741	-10.688	1.00	37.15
4114	O	THR	B	43	-26.862	-18.883	-10.994	1.00	35.8
4115	CB	THR	B	43	-24.705	-16.561	-11.886	1.00	37.05
4116	OG1	THR	B	43	-25.238	-17.236	-13.035	1.00	38.07
4117	CG2	THR	B	43	-23.197	-16.394	-12.044	1.00	36.87
4118	N	CYS	B	44	-27.368	-16.768	-10.405	1.00	37.6
4119	CA	CYS	B	44	-28.799	-17.004	-10.449	1.00	38.55

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

4120	C	CYS	B	44	-29.2	-17.371	-11.872	1.00	38.16
4121	O	CYS	B	44	-29.956	-18.315	-12.085	1.00	39.1
4122	CB	CYS	B	44	-29.564	-15.762	-9.969	1.00	39.19
4123	SG	CYS	B	44	-29.393	-15.411	-8.183	1.00	41.48
4124	N	ALA	B	45	-28.679	-16.632	-12.844	1.00	37.64
4125	CA	ALA	B	45	-28.984	-16.899	-14.247	1.00	37.74
4126	C	ALA	B	45	-28.661	-18.35	-14.609	1.00	37.41
4127	O	ALA	B	45	-29.395	-18.986	-15.366	1.00	37.06
4128	CB	ALA	B	45	-28.196	-15.943	-15.148	1.00	35.75
4129	N	GLU	B	46	-27.559	-18.865	-14.068	1.00	37.98
4130	CA	GLU	B	46	-27.143	-20.241	-14.334	1.00	38.45
4131	C	GLU	B	46	-28.155	-21.256	-13.819	1.00	37.68
4132	O	GLU	B	46	-28.325	-22.322	-14.408	1.00	39.59
4133	CB	GLU	B	46	-25.79	-20.534	-13.684	1.00	41.05
4134	CG	GLU	B	46	-24.58	-19.994	-14.414	1.00	43.22
4135	CD	GLU	B	46	-23.28	-20.376	-13.719	1.00	45.63
4136	OE1	GLU	B	46	-23.065	-19.923	-12.572	1.00	45.54
4137	OE2	GLU	B	46	-22.48	-21.133	-14.314	1.00	46.58
4138	N	LEU	B	47	-28.816	-20.93	-12.713	1.00	35.79
4139	CA	LEU	B	47	-29.806	-21.827	-12.128	1.00	33.77
4140	C	LEU	B	47	-31.077	-21.88	-12.969	1.00	33.48
4141	O	LEU	B	47	-31.667	-22.947	-13.145	1.00	32.34
4142	CB	LEU	B	47	-30.154	-21.378	-10.707	1.00	32.42
4143	CG	LEU	B	47	-29.029	-21.429	-9.677	1.00	30.14
4144	CD1	LEU	B	47	-29.54	-20.892	-8.347	1.00	29.98
4145	CD2	LEU	B	47	-28.531	-22.86	-9.535	1.00	28.93
4146	N	TYR	B	48	-31.499	-20.723	-13.475	1.00	33.9
4147	CA	TYR	B	48	-32.697	-20.643	-14.304	1.00	33.93
4148	C	TYR	B	48	-32.531	-21.503	-15.544	1.00	34.35
4149	O	TYR	B	48	-33.506	-21.936	-16.148	1.00	34.79
4150	CB	TYR	B	48	-32.964	-19.2	-14.744	1.00	33.81
4151	CG	TYR	B	48	-33.75	-18.362	-13.761	1.00	34.55
4152	CD1	TYR	B	48	-33.107	-17.542	-12.831	1.00	33.57
4153	CD2	TYR	B	48	-35.146	-18.389	-13.762	1.00	33.93
4154	CE1	TYR	B	48	-33.84	-16.765	-11.927	1.00	33.14
4155	CE2	TYR	B	48	-35.885	-17.621	-12.865	1.00	33.56
4156	CZ	TYR	B	48	-35.228	-16.813	-11.952	1.00	33.1
4157	OH	TYR	B	48	-35.967	-16.061	-11.07	1.00	32.28
4158	N	GLU	B	49	-31.285	-21.747	-15.923	1.00	35.29
4159	CA	GLU	B	49	-30.997	-22.538	-17.108	1.00	36.53

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

4160	C	GLU	B	49	-30.788	-24.02	-16.809	1.00	35.79
4161	O	GLU	B	49	-31.372	-24.879	-17.467	1.00	34.72
4162	CB	GLU	B	49	-29.754	-21.977	-17.803	1.00	38.73
4163	CG	GLU	B	49	-29.287	-22.784	-19.002	1.00	43.29
4164	CD	GLU	B	49	-27.941	-22.316	-19.526	1.00	45.75
4165	OE1	GLU	B	49	-26.926	-22.482	-18.814	1.00	47.27
4166	OE2	GLU	B	49	-27.899	-21.777	-20.649	1.00	48.35
4167	N	LYS	B	50	-29.957	-24.311	-15.812	1.00	35.03
4168	CA	LYS	B	50	-29.644	-25.692	-15.455	1.00	34.64
4169	C	LYS	B	50	-30.729	-26.483	-14.733	1.00	33.92
4170	O	LYS	B	50	-31.017	-27.619	-15.114	1.00	33.45
4171	CB	LYS	B	50	-28.356	-25.734	-14.631	1.00	34.99
4172	CG	LYS	B	50	-27.101	-25.411	-15.427	1.00	36.88
4173	CD	LYS	B	50	-25.864	-25.433	-14.541	1.00	39.4
4174	CE	LYS	B	50	-24.587	-25.335	-15.363	1.00	42.32
4175	NZ	LYS	B	50	-24.545	-24.101	-16.202	1.00	44.34
4176	N	LEU	B	51	-31.324	-25.895	-13.696	1.00	32.94
4177	CA	LEU	B	51	-32.359	-26.581	-12.925	1.00	33.89
4178	C	LEU	B	51	-33.419	-27.258	-13.797	1.00	34.77
4179	O	LEU	B	51	-33.719	-28.439	-13.619	1.00	34.81
4180	CB	LEU	B	51	-33.03	-25.612	-11.943	1.00	32.92
4181	CG	LEU	B	51	-32.169	-25.109	-10.776	1.00	33.7
4182	CD1	LEU	B	51	-32.937	-24.056	-9.998	1.00	33.18
4183	CD2	LEU	B	51	-31.783	-26.269	-9.867	1.00	31.66
4184	N	PRO	B	52	-34.001	-26.518	-14.751	1.00	35.49
4185	CA	PRO	B	52	-35.024	-27.109	-15.619	1.00	35.41
4186	C	PRO	B	52	-34.496	-28.294	-16.428	1.00	34.91
4187	O	PRO	B	52	-35.266	-29.148	-16.86	1.00	34.39
4188	CB	PRO	B	52	-35.435	-25.937	-16.505	1.00	36.06
4189	CG	PRO	B	52	-35.242	-24.756	-15.597	1.00	35.58
4190	CD	PRO	B	52	-33.901	-25.066	-14.983	1.00	35.05
4191	N	GLN	B	53	-33.181	-28.34	-16.616	1.00	34.77
4192	CA	GLN	B	53	-32.541	-29.409	-17.378	1.00	35.04
4193	C	GLN	B	53	-32.249	-30.65	-16.54	1.00	34.67
4194	O	GLN	B	53	-31.784	-31.668	-17.066	1.00	34.73
4195	CB	GLN	B	53	-31.243	-28.895	-17.989	1.00	37.1
4196	CG	GLN	B	53	-31.438	-27.71	-18.916	1.00	41.57
4197	CD	GLN	B	53	-30.132	-27.014	-19.257	1.00	44.49
4198	OE1	GLN	B	53	-30.106	-26.089	-20.071	1.00	46.84
4199	NE2	GLN	B	53	-29.041	-27.452	-18.63	1.00	43.94

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

4200	N	GLY	B	54	-32.508	-30.564	-15.238	1.00	33.05
4201	CA	GLY	B	54	-32.275	-31.702	-14.372	1.00	29.91
4202	C	GLY	B	54	-31.187	-31.51	-13.334	1.00	29.62
4203	O	GLY	B	54	-31.005	-32.361	-12.464	1.00	30.24
4204	N	TYR	B	55	-30.463	-30.401	-13.403	1.00	27.63
4205	CA	TYR	B	55	-29.401	-30.163	-12.435	1.00	27.14
4206	C	TYR	B	55	-29.938	-29.972	-11.018	1.00	25.73
4207	O	TYR	B	55	-30.943	-29.285	-10.808	1.00	25.31
4208	CB	TYR	B	55	-28.569	-28.943	-12.838	1.00	26.83
4209	CG	TYR	B	55	-27.424	-28.674	-11.894	1.00	27.47
4210	CD1	TYR	B	55	-27.627	-27.987	-10.698	1.00	27.06
4211	CD2	TYR	B	55	-26.143	-29.15	-12.17	1.00	27.25
4212	CE1	TYR	B	55	-26.591	-27.781	-9.801	1.00	26.54
4213	CE2	TYR	B	55	-25.096	-28.95	-11.278	1.00	28.14
4214	CZ	TYR	B	55	-25.33	-28.263	-10.093	1.00	28.26
4215	OH	TYR	B	55	-24.305	-28.054	-9.201	1.00	28.83
4216	N	ARG	B	56	-29.254	-30.577	-10.051	1.00	23.8
4217	CA	ARG	B	56	-29.643	-30.482	-8.647	1.00	23.35
4218	C	ARG	B	56	-28.415	-30.338	-7.754	1.00	23.69
4219	O	ARG	B	56	-27.317	-30.735	-8.136	1.00	25.04
4220	CB	ARG	B	56	-30.423	-31.732	-8.23	1.00	22.27
4221	CG	ARG	B	56	-31.758	-31.938	-8.953	1.00	21.24
4222	CD	ARG	B	56	-32.795	-30.891	-8.552	1.00	18.77
4223	NE	ARG	B	56	-34.102	-31.17	-9.147	1.00	21.29
4224	CZ	ARG	B	56	-34.437	-30.903	-10.41	1.00	18.94
4225	NH1	ARG	B	56	-33.566	-30.335	-11.233	1.00	15.48
4226	NH2	ARG	B	56	-35.645	-31.218	-10.853	1.00	16.53
4227	N	LEU	B	57	-28.601	-29.76	-6.569	1.00	23.86
4228	CA	LEU	B	57	-27.508	-29.588	-5.618	1.00	23.35
4229	C	LEU	B	57	-26.777	-30.911	-5.394	1.00	24.84
4230	O	LEU	B	57	-27.396	-31.976	-5.318	1.00	25.15
4231	CB	LEU	B	57	-28.05	-29.093	-4.274	1.00	22.79
4232	CG	LEU	B	57	-28.468	-27.628	-4.153	1.00	24.23
4233	CD1	LEU	B	57	-29.382	-27.45	-2.95	1.00	23.15
4234	CD2	LEU	B	57	-27.228	-26.753	-4.022	1.00	23.46
4235	N	GLU	B	58	-25.457	-30.846	-5.281	1.00	25.16
4236	CA	GLU	B	58	-24.673	-32.05	-5.05	1.00	26.53
4237	C	GLU	B	58	-24.771	-32.455	-3.58	1.00	24.07
4238	O	GLU	B	58	-25.071	-31.626	-2.721	1.00	22.34
4239	CB	GLU	B	58	-23.214	-31.81	-5.466	1.00	31.4

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

4240	CG	GLU	B	58	-23.014	-31.859	-6.987	1.00	39.35
4241	CD	GLU	B	58	-21.966	-30.875	-7.493	1.00	44.78
4242	OE1	GLU	B	58	-20.76	-31.066	-7.214	1.00	47.94
4243	OE2	GLU	B	58	-22.359	-29.9	-8.175	1.00	47.62
4244	N	LYS	B	59	-24.54	-33.733	-3.297	1.00	21.65
4245	CA	LYS	B	59	-24.618	-34.222	-1.929	1.00	22.02
4246	C	LYS	B	59	-23.469	-33.732	-1.064	1.00	21.17
4247	O	LYS	B	59	-22.303	-33.886	-1.423	1.00	21.73
4248	CB	LYS	B	59	-24.623	-35.75	-1.891	1.00	22.3
4249	CG	LYS	B	59	-24.686	-36.302	-0.47	1.00	24.58
4250	CD	LYS	B	59	-24.674	-37.821	-0.438	1.00	29.11
4251	CE	LYS	B	59	-23.334	-38.372	-0.894	1.00	32.27
4252	NZ	LYS	B	59	-23.336	-39.859	-0.968	1.00	35.57
4253	N	PRO	B	60	-23.783	-33.126	0.09	1.00	20.94
4254	CA	PRO	B	60	-22.71	-32.646	0.963	1.00	20.41
4255	C	PRO	B	60	-21.789	-33.827	1.278	1.00	20.86
4256	O	PRO	B	60	-22.226	-34.983	1.291	1.00	21.17
4257	CB	PRO	B	60	-23.465	-32.141	2.191	1.00	21.27
4258	CG	PRO	B	60	-24.758	-31.656	1.601	1.00	20.46
4259	CD	PRO	B	60	-25.107	-32.76	0.625	1.00	19.65
4260	N	LEU	B	61	-20.519	-33.533	1.528	1.00	21.03
4261	CA	LEU	B	61	-19.526	-34.563	1.806	1.00	19.82
4262	C	LEU	B	61	-19.73	-35.344	3.105	1.00	18.79
4263	O	LEU	B	61	-19.276	-36.477	3.22	1.00	21.09
4264	CB	LEU	B	61	-18.13	-33.93	1.78	1.00	19.58
4265	CG	LEU	B	61	-17.763	-33.269	0.436	1.00	20.63
4266	CD1	LEU	B	61	-16.355	-32.669	0.511	1.00	19.99
4267	CD2	LEU	B	61	-17.826	-34.305	-0.686	1.00	16.3
4268	N	ASN	B	62	-20.424	-34.749	4.07	1.00	16.02
4269	CA	ASN	B	62	-20.676	-35.386	5.365	1.00	15.04
4270	C	ASN	B	62	-22.116	-35.908	5.438	1.00	16.25
4271	O	ASN	B	62	-22.634	-36.174	6.524	1.00	16.62
4272	CB	ASN	B	62	-20.503	-34.349	6.46	1.00	12.63
4273	CG	ASN	B	62	-21.558	-33.269	6.374	1.00	12.41
4274	OD1	ASN	B	62	-21.904	-32.817	5.277	1.00	13.08
4275	ND2	ASN	B	62	-22.084	-32.858	7.513	1.00	11.74
4276	N	CYS	B	63	-22.759	-36.044	4.285	1.00	16.99
4277	CA	CYS	B	63	-24.149	-36.477	4.224	1.00	17.96
4278	C	CYS	B	63	-24.337	-37.944	3.864	1.00	17.58
4279	O	CYS	B	63	-23.749	-38.438	2.904	1.00	17.21

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## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

4280	CB	CYS	B	63	-24.897	-35.598	3.213	1.00	18.99
4281	SG	CYS	B	63	-26.694	-35.801	3.163	1.00	19.06
4282	N	ASP	B	64	-25.171	-38.633	4.639	1.00	18.5
4283	CA	ASP	B	64	-25.461	-40.044	4.391	1.00	18.73
4284	C	ASP	B	64	-26.357	-40.148	3.155	1.00	18.54
4285	O	ASP	B	64	-27.187	-39.278	2.909	1.00	18.54
4286	CB	ASP	B	64	-26.177	-40.657	5.596	1.00	20.91
4287	CG	ASP	B	64	-26.487	-42.129	5.404	1.00	24.15
4288	OD1	ASP	B	64	-25.585	-42.963	5.63	1.00	27.24
4289	OD2	ASP	B	64	-27.629	-42.453	5.014	1.00	25.59
4290	N	ASP	B	65	-26.189	-41.208	2.377	1.00	19.27
4291	CA	ASP	B	65	-26.995	-41.395	1.175	1.00	19.48
4292	C	ASP	B	65	-28.502	-41.274	1.392	1.00	18.6
4293	O	ASP	B	65	-29.21	-40.774	0.52	1.00	18.86
4294	CB	ASP	B	65	-26.719	-42.763	0.537	1.00	21.3
4295	CG	ASP	B	65	-25.452	-42.783	-0.285	1.00	23.39
4296	OD1	ASP	B	65	-25.122	-41.744	-0.895	1.00	26.26
4297	OD2	ASP	B	65	-24.799	-43.847	-0.339	1.00	25.45
4298	N	GLU	B	66	-29.006	-41.735	2.535	1.00	17.38
4299	CA	GLU	B	66	-30.447	-41.666	2.755	1.00	17.26
4300	C	GLU	B	66	-30.971	-40.241	2.923	1.00	16.17
4301	O	GLU	B	66	-32.059	-39.924	2.456	1.00	16.56
4302	CB	GLU	B	66	-30.867	-42.513	3.958	1.00	17.34
4303	CG	GLU	B	66	-32.287	-43.027	3.814	1.00	18.15
4304	CD	GLU	B	66	-32.834	-43.667	5.076	1.00	18.5
4305	OE1	GLU	B	66	-32.063	-44.323	5.808	1.00	17.05
4306	OE2	GLU	B	66	-34.051	-43.522	5.321	1.00	17.96
4307	N	VAL	B	67	-30.202	-39.383	3.585	1.00	15.38
4308	CA	VAL	B	67	-30.629	-38.004	3.774	1.00	15.26
4309	C	VAL	B	67	-30.63	-37.319	2.415	1.00	15.72
4310	O	VAL	B	67	-31.548	-36.567	2.083	1.00	16.3
4311	CB	VAL	B	67	-29.687	-37.228	4.735	1.00	15.28
4312	CG1	VAL	B	67	-30.222	-35.828	4.972	1.00	10.67
4313	CG2	VAL	B	67	-29.562	-37.97	6.06	1.00	13.93
4314	N	TYR	B	68	-29.606	-37.593	1.617	1.00	15.7
4315	CA	TYR	B	68	-29.526	-36.98	0.301	1.00	15.71
4316	C	TYR	B	68	-30.704	-37.405	-0.562	1.00	15.98
4317	O	TYR	B	68	-31.254	-36.601	-1.317	1.00	14.87
4318	CB	TYR	B	68	-28.212	-37.356	-0.391	1.00	15.02
4319	CG	TYR	B	68	-28.003	-36.64	-1.712	1.00	14.72

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## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

4320	CD1	TYR	B	68	-28.011	-35.24	-1.778	1.00	12.2
4321	CD2	TYR	B	68	-27.815	-37.36	-2.901	1.00	13.12
4322	CE1	TYR	B	68	-27.841	-34.573	-2.997	1.00	12.28
4323	CE2	TYR	B	68	-27.645	-36.703	-4.127	1.00	12.71
4324	CZ	TYR	B	68	-27.663	-35.313	-4.167	1.00	12.96
4325	OH	TYR	B	68	-27.537	-34.661	-5.369	1.00	10.57
4326	N	ASP	B	69	-31.092	-38.671	-0.448	1.00	17.93
4327	CA	ASP	B	69	-32.208	-39.195	-1.231	1.00	20.68
4328	C	ASP	B	69	-33.489	-38.432	-0.879	1.00	20.37
4329	O	ASP	B	69	-34.334	-38.164	-1.744	1.00	20.21
4330	CB	ASP	B	69	-32.386	-40.694	-0.959	1.00	24.34
4331	CG	ASP	B	69	-33.436	-41.332	-1.858	1.00	29.69
4332	OD1	ASP	B	69	-33.277	-41.257	-3.095	1.00	32.41
4333	OD2	ASP	B	69	-34.42	-41.905	-1.334	1.00	31.87
4334	N	LEU	B	70	-33.625	-38.085	0.397	1.00	17.65
4335	CA	LEU	B	70	-34.776	-37.34	0.866	1.00	14.39
4336	C	LEU	B	70	-34.775	-35.974	0.187	1.00	14.21
4337	O	LEU	B	70	-35.819	-35.492	-0.254	1.00	15.84
4338	CB	LEU	B	70	-34.706	-37.185	2.383	1.00	15.2
4339	CG	LEU	B	70	-35.834	-36.42	3.075	1.00	14.04
4340	CD1	LEU	B	70	-37.175	-37.06	2.705	1.00	14.6
4341	CD2	LEU	B	70	-35.617	-36.456	4.591	1.00	13.9
4342	N	MET	B	71	-33.605	-35.346	0.107	1.00	13.26
4343	CA	MET	B	71	-33.482	-34.045	-0.553	1.00	13.45
4344	C	MET	B	71	-33.937	-34.167	-2.005	1.00	13.49
4345	O	MET	B	71	-34.724	-33.36	-2.503	1.00	12.4
4346	CB	MET	B	71	-32.026	-33.564	-0.552	1.00	13.06
4347	CG	MET	B	71	-31.499	-33.099	0.782	1.00	11.68
4348	SD	MET	B	71	-29.775	-32.605	0.647	1.00	16.08
4349	CE	MET	B	71	-29.048	-33.468	2.108	1.00	12.57
4350	N	ARG	B	72	-33.426	-35.187	-2.682	1.00	14.13
4351	CA	ARG	B	72	-33.77	-35.409	-4.075	1.00	16.56
4352	C	ARG	B	72	-35.28	-35.57	-4.282	1.00	17.55
4353	O	ARG	B	72	-35.841	-34.994	-5.216	1.00	17.31
4354	CB	ARG	B	72	-33.001	-36.621	-4.609	1.00	17.35
4355	CG	ARG	B	72	-31.486	-36.413	-4.646	1.00	16.9
4356	CD	ARG	B	72	-31.126	-35.212	-5.508	1.00	17.83
4357	NE	ARG	B	72	-31.539	-35.411	-6.899	1.00	20.95
4358	CZ	ARG	B	72	-30.704	-35.681	-7.901	1.00	20.17
4359	NH1	ARG	B	72	-29.401	-35.778	-7.678	1.00	18.29



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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

4360	NH2	ARG	B	72	-31.175	-35.874	-9.127	1.00	21.39
4361	N	GLN	B	73	-35.938	-36.338	-3.415	1.00	17.55
4362	CA	GLN	B	73	-37.386	-36.512	-3.519	1.00	17.42
4363	C	GLN	B	73	-38.072	-35.139	-3.52	1.00	17.14
4364	O	GLN	B	73	-39.018	-34.905	-4.279	1.00	16.33
4365	CB	GLN	B	73	-37.94	-37.303	-2.334	1.00	18.29
4366	CG	GLN	B	73	-37.425	-38.711	-2.149	1.00	23.82
4367	CD	GLN	B	73	-38.019	-39.367	-0.895	1.00	27.36
4368	OE1	GLN	B	73	-37.413	-40.263	-0.298	1.00	26.86
4369	NE2	GLN	B	73	-39.213	-38.921	-0.5	1.00	26.99
4370	N	CYS	B	74	-37.588	-34.242	-2.659	1.00	15.16
4371	CA	CYS	B	74	-38.149	-32.9	-2.534	1.00	15.66
4372	C	CYS	B	74	-38.008	-32.06	-3.8	1.00	16.23
4373	O	CYS	B	74	-38.812	-31.151	-4.026	1.00	15.19
4374	CB	CYS	B	74	-37.504	-32.147	-1.358	1.00	15.96
4375	SG	CYS	B	74	-37.869	-32.806	0.317	1.00	15.36
4376	N	TRP	B	75	-37.005	-32.367	-4.627	1.00	16.37
4377	CA	TRP	B	75	-36.779	-31.611	-5.853	1.00	16.39
4378	C	TRP	B	75	-37.184	-32.321	-7.141	1.00	18.27
4379	O	TRP	B	75	-36.641	-32.018	-8.208	1.00	17.49
4380	CB	TRP	B	75	-35.312	-31.207	-5.98	1.00	16.65
4381	CG	TRP	B	75	-34.745	-30.607	-4.759	1.00	17.24
4382	CD1	TRP	B	75	-35.339	-29.693	-3.938	1.00	17.52
4383	CD2	TRP	B	75	-33.452	-30.863	-4.211	1.00	16.49
4384	NE1	TRP	B	75	-34.494	-29.365	-2.909	1.00	18.01
4385	CE2	TRP	B	75	-33.327	-30.069	-3.051	1.00	16.63
4386	CE3	TRP	B	75	-32.384	-31.688	-4.588	1.00	17.13
4387	CZ2	TRP	B	75	-32.176	-30.072	-2.26	1.00	15.61
4388	CZ3	TRP	B	75	-31.237	-31.692	-3.804	1.00	16.75
4389	CH2	TRP	B	75	-31.145	-30.885	-2.649	1.00	17.46
4390	N	ARG	B	76	-38.111	-33.269	-7.048	1.00	19.53
4391	CA	ARG	B	76	-38.585	-33.972	-8.235	1.00	21.36
4392	C	ARG	B	76	-39.284	-32.937	-9.106	1.00	22.58
4393	O	ARG	B	76	-39.983	-32.055	-8.593	1.00	21.15
4394	CB	ARG	B	76	-39.563	-35.087	-7.845	1.00	22.54
4395	CG	ARG	B	76	-38.888	-36.358	-7.363	1.00	24.98
4396	CD	ARG	B	76	-39.803	-37.18	-6.478	1.00	28.53
4397	NE	ARG	B	76	-39.196	-38.458	-6.109	1.00	31.18
4398	CZ	ARG	B	76	-39.632	-39.242	-5.124	1.00	31.91
4399	NH1	ARG	B	76	-39.012	-40.39	-4.865	1.00	31.83

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TABLE 3

STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

4400	NH2	ARG	B	76	-40.677	-38.875	-4.389	1.00	29.49
4401	N	GLU	B	77	-39.092	-33.043	-10.418	1.00	24.71
4402	CA	GLU	B	77	-39.683	-32.095	-11.358	1.00	27.93
4403	C	GLU	B	77	-41.195	-31.985	-11.236	1.00	27.63
4404	O	GLU	B	77	-41.735	-30.854	-11.285	1.00	26.42
4405	CB	GLU	B	77	-39.318	-32.479	-12.79	1.00	30.64
4406	CG	GLU	B	77	-39.686	-31.427	-13.82	1.00	37.57
4407	CD	GLU	B	77	-38.991	-31.66	-15.158	1.00	43.77
4408	OE1	GLU	B	77	-37.737	-31.688	-15.184	1.00	46.11
4409	OE2	GLU	B	77	-39.693	-31.816	-16.183	1.00	45.51
4410	N	LYS	B	78	-41.879	-33.092	-11.085	1.00	27.42
4411	CA	LYS	B	78	-43.329	-33.076	-10.957	1.00	29.28
4412	C	LYS	B	78	-43.695	-32.768	-9.513	1.00	28.69
4413	O	LYS	B	78	-43.484	-33.591	-8.62	1.00	29.44
4414	CB	LYS	B	78	-43.912	-34.424	-11.373	1.00	31.27
4415	CG	LYS	B	78	-43.634	-34.78	-12.828	1.00	34.35
4416	CD	LYS	B	78	-44.106	-36.193	-13.126	1.00	37.45
4417	CE	LYS	B	78	-43.718	-36.638	-14.519	1.00	38.57
4418	NZ	LYS	B	78	-44.042	-38.085	-14.705	1.00	41.72
4419	N	PRO	B	79	-44.257	-31.574	-9.27	1.00	26.9
4420	CA	PRO	B	79	-44.66	-31.12	-7.936	1.00	26.3
4421	C	PRO	B	79	-45.48	-32.138	-7.144	1.00	27.1
4422	O	PRO	B	79	-45.32	-32.265	-5.926	1.00	26.74
4423	CB	PRO	B	79	-45.452	-29.845	-8.23	1.00	25.83
4424	CG	PRO	B	79	-44.831	-29.34	-9.486	1.00	25.17
4425	CD	PRO	B	79	-44.672	-30.603	-10.297	1.00	25.18
4426	N	TYR	B	80	-46.357	-32.86	-7.836	1.00	26.64
4427	CA	TYR	B	80	-47.205	-33.846	-7.177	1.00	27.58
4428	C	TYR	B	80	-46.482	-35.134	-6.8	1.00	26.97
4429	O	TYR	B	80	-47.037	-35.966	-6.087	1.00	28.21
4430	CB	TYR	B	80	-48.429	-34.161	-8.049	1.00	29.45
4431	CG	TYR	B	80	-48.105	-34.447	-9.501	1.00	31.82
4432	CD1	TYR	B	80	-47.775	-35.737	-9.926	1.00	32.41
4433	CD2	TYR	B	80	-48.115	-33.421	-10.449	1.00	31.47
4434	CE1	TYR	B	80	-47.466	-35.999	-11.26	1.00	33.19
4435	CE2	TYR	B	80	-47.809	-33.667	-11.779	1.00	33.46
4436	CZ	TYR	B	80	-47.486	-34.958	-12.181	1.00	35.29
4437	OH	TYR	B	80	-47.185	-35.202	-13.505	1.00	36.69
4438	N	GLU	B	81	-45.249	-35.303	-7.269	1.00	25.56
4439	CA	GLU	B	81	-44.485	-36.5	-6.935	1.00	24.88

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

4440	C	GLU	B	81	-43.603	-36.276	-5.705	1.00	23.83
4441	O	GLU	B	81	-43.026	-37.216	-5.154	1.00	23.55
4442	CB	GLU	B	81	-43.625	-36.947	-8.123	1.00	26.69
4443	CG	GLU	B	81	-44.443	-37.397	-9.328	1.00	30.4
4444	CD	GLU	B	81	-43.633	-38.184	-10.343	1.00	31.67
4445	OE1	GLU	B	81	-42.584	-37.683	-10.813	1.00	32.36
4446	OE2	GLU	B	81	-44.059	-39.309	-10.679	1.00	33.81
4447	N	ARG	B	82	-43.497	-35.028	-5.268	1.00	20.62
4448	CA	ARG	B	82	-42.693	-34.737	-4.097	1.00	19.52
4449	C	ARG	B	82	-43.391	-35.32	-2.88	1.00	19.04
4450	O	ARG	B	82	-44.601	-35.55	-2.893	1.00	19.33
4451	CB	ARG	B	82	-42.52	-33.226	-3.93	1.00	18.38
4452	CG	ARG	B	82	-41.731	-32.588	-5.067	1.00	17.1
4453	CD	ARG	B	82	-41.895	-31.082	-5.12	1.00	15.52
4454	NE	ARG	B	82	-41.39	-30.568	-6.388	1.00	18.93
4455	CZ	ARG	B	82	-41.574	-29.329	-6.838	1.00	19.2
4456	NH1	ARG	B	82	-42.251	-28.445	-6.117	1.00	15.76
4457	NH2	ARG	B	82	-41.116	-28.991	-8.039	1.00	18.81
4458	N	PRO	B	83	-42.629	-35.609	-1.82	1.00	17.8
4459	CA	PRO	B	83	-43.28	-36.161	-0.636	1.00	17.24
4460	C	PRO	B	83	-44.056	-35.059	0.069	1.00	17.22
4461	O	PRO	B	83	-43.861	-33.873	-0.208	1.00	16.73
4462	CB	PRO	B	83	-42.106	-36.654	0.198	1.00	17.42
4463	CG	PRO	B	83	-41.022	-35.674	-0.15	1.00	17.17
4464	CD	PRO	B	83	-41.167	-35.576	-1.651	1.00	17.9
4465	N	SER	B	84	-44.946	-35.452	0.968	1.00	16.45
4466	CA	SER	B	84	-45.709	-34.482	1.738	1.00	15.02
4467	C	SER	B	84	-44.87	-34.246	2.99	1.00	13.54
4468	O	SER	B	84	-43.976	-35.039	3.3	1.00	13.3
4469	CB	SER	B	84	-47.06	-35.063	2.143	1.00	12.05
4470	OG	SER	B	84	-46.863	-36.155	3.026	1.00	16.71
4471	N	PHE	B	85	-45.155	-33.175	3.715	1.00	11.89
4472	CA	PHE	B	85	-44.401	-32.897	4.924	1.00	12.26
4473	C	PHE	B	85	-44.543	-34.008	5.953	1.00	12.41
4474	O	PHE	B	85	-43.588	-34.317	6.666	1.00	12.49
4475	CB	PHE	B	85	-44.816	-31.543	5.509	1.00	10.66
4476	CG	PHE	B	85	-44.166	-30.382	4.825	1.00	9.45
4477	CD1	PHE	B	85	-42.781	-30.203	4.899	1.00	7.1
4478	CD2	PHE	B	85	-44.924	-29.475	4.082	1.00	9.86
4479	CE1	PHE	B	85	-42.157	-29.133	4.239	1.00	7.97

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

4480	CE2	PHE	B	85	-44.308	-28.399	3.417	1.00	9.92
4481	CZ	PHE	B	85	-42.918	-28.231	3.498	1.00	7.31
4482	N	ALA	B	86	-45.722	-34.62	6.024	1.00	13.41
4483	CA	ALA	B	86	-45.945	-35.721	6.966	1.00	14.28
4484	C	ALA	B	86	-45.011	-36.888	6.627	1.00	15.75
4485	O	ALA	B	86	-44.432	-37.51	7.52	1.00	17.28
4486	CB	ALA	B	86	-47.408	-36.185	6.911	1.00	13.65
4487	N	GLN	B	87	-44.858	-37.181	5.338	1.00	15.14
4488	CA	GLN	B	87	-43.98	-38.272	4.926	1.00	16.49
4489	C	GLN	B	87	-42.533	-37.936	5.267	1.00	17.04
4490	O	GLN	B	87	-41.797	-38.792	5.77	1.00	19.49
4491	CB	GLN	B	87	-44.111	-38.545	3.419	1.00	16.92
4492	CG	GLN	B	87	-45.496	-39.005	2.988	1.00	16.37
4493	CD	GLN	B	87	-45.62	-39.139	1.483	1.00	19.67
4494	OE1	GLN	B	87	-45.279	-38.22	0.735	1.00	20.94
4495	NE2	GLN	B	87	-46.118	-40.283	1.03	1.00	19.24
4496	N	ILE	B	88	-42.122	-36.695	5.003	1.00	14.99
4497	CA	ILE	B	88	-40.757	-36.278	5.312	1.00	14.37
4498	C	ILE	B	88	-40.488	-36.474	6.808	1.00	14.68
4499	O	ILE	B	88	-39.393	-36.877	7.199	1.00	17.24
4500	CB	ILE	B	88	-40.509	-34.788	4.913	1.00	14.09
4501	CG1	ILE	B	88	-40.583	-34.639	3.388	1.00	13.63
4502	CG2	ILE	B	88	-39.146	-34.323	5.394	1.00	9.19
4503	CD1	ILE	B	88	-40.485	-33.193	2.902	1.00	11.47
4504	N	LEU	B	89	-41.485	-36.211	7.645	1.00	12.6
4505	CA	LEU	B	89	-41.301	-36.383	9.08	1.00	14.79
4506	C	LEU	B	89	-41.164	-37.861	9.468	1.00	15.85
4507	O	LEU	B	89	-40.417	-38.2	10.396	1.00	13.77
4508	CB	LEU	B	89	-42.463	-35.747	9.847	1.00	15.76
4509	CG	LEU	B	89	-42.325	-35.783	11.372	1.00	17.67
4510	CD1	LEU	B	89	-40.988	-35.182	11.776	1.00	17.12
4511	CD2	LEU	B	89	-43.475	-35.022	12.013	1.00	16.76
4512	N	VAL	B	90	-41.885	-38.739	8.767	1.00	16
4513	CA	VAL	B	90	-41.808	-40.174	9.051	1.00	15.29
4514	C	VAL	B	90	-40.407	-40.676	8.704	1.00	15.85
4515	O	VAL	B	90	-39.799	-41.421	9.47	1.00	13.73
4516	CB	VAL	B	90	-42.877	-40.976	8.252	1.00	15.62
4517	CG1	VAL	B	90	-42.509	-42.457	8.213	1.00	12.4
4518	CG2	VAL	B	90	-44.251	-40.802	8.912	1.00	8.4
4519	N	SER	B	91	-39.885	-40.243	7.562	1.00	16.02

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

4520	CA	SER	B	91	-38.544	-40.646	7.153	1.00	16.23
4521	C	SER	B	91	-37.515	-40.208	8.198	1.00	17.32
4522	O	SER	B	91	-36.75	-41.025	8.7	1.00	18.56
4523	CB	SER	B	91	-38.194	-40.02	5.807	1.00	15.2
4524	OG	SER	B	91	-39.142	-40.379	4.824	1.00	16.89
4525	N	LEU	B	92	-37.501	-38.916	8.517	1.00	17.05
4526	CA	LEU	B	92	-36.569	-38.379	9.508	1.00	18.4
4527	C	LEU	B	92	-36.705	-39.071	10.866	1.00	18.86
4528	O	LEU	B	92	-35.708	-39.308	11.552	1.00	17.77
4529	CB	LEU	B	92	-36.788	-36.871	9.696	1.00	17.21
4530	CG	LEU	B	92	-36.402	-35.963	8.531	1.00	16.81
4531	CD1	LEU	B	92	-36.983	-34.564	8.738	1.00	14.17
4532	CD2	LEU	B	92	-34.884	-35.923	8.415	1.00	15.69
4533	N	ASN	B	93	-37.932	-39.39	11.266	1.00	18.27
4534	CA	ASN	B	93	-38.111	-40.052	12.551	1.00	17.66
4535	C	ASN	B	93	-37.541	-41.463	12.548	1.00	18.57
4536	O	ASN	B	93	-37.071	-41.948	13.585	1.00	18.76
4537	CB	ASN	B	93	-39.586	-40.078	12.958	1.00	15.87
4538	CG	ASN	B	93	-40.067	-38.731	13.485	1.00	16.37
4539	OD1	ASN	B	93	-39.202	-37.864	13.825	1.00	15.56
4540	ND2	ASN	B	93	-41.377	-38.561	13.572	1.00	14.99
4541	N	ARG	B	94	-37.561	-42.124	11.39	1.00	17.77
4542	CA	ARG	B	94	-37.026	-43.477	11.32	1.00	18.57
4543	C	ARG	B	94	-35.518	-43.384	11.541	1.00	19.99
4544	O	ARG	B	94	-34.939	-44.185	12.28	1.00	19.45
4545	CB	ARG	B	94	-37.337	-44.132	9.959	1.00	18.34
4546	CG	ARG	B	94	-38.756	-43.883	9.475	1.00	18.22
4547	CD	ARG	B	94	-39.607	-45.131	9.29	1.00	16.81
4548	NE	ARG	B	94	-39.597	-45.594	7.904	1.00	15.66
4549	CZ	ARG	B	94	-40.557	-46.325	7.341	1.00	14.26
4550	NH1	ARG	B	94	-41.626	-46.69	8.035	1.00	11.96
4551	NH2	ARG	B	94	-40.445	-46.694	6.071	1.00	14.25
4552	N	MET	B	95	-34.888	-42.389	10.918	1.00	19.87
4553	CA	MET	B	95	-33.45	-42.202	11.07	1.00	20.03
4554	C	MET	B	95	-33.083	-41.788	12.493	1.00	20.31
4555	O	MET	B	95	-32.062	-42.214	13.021	1.00	22.95
4556	CB	MET	B	95	-32.934	-41.175	10.056	1.00	20.71
4557	CG	MET	B	95	-33.033	-41.651	8.604	1.00	22.66
4558	SD	MET	B	95	-32.334	-40.502	7.373	1.00	25.9
4559	CE	MET	B	95	-33.749	-39.5	6.974	1.00	22.78

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TABLE 3

STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

4560	N	LEU	B	96	-33.915	-40.968	13.122	1.00	21.14
4561	CA	LEU	B	96	-33.649	-40.533	14.494	1.00	22.8
4562	C	LEU	B	96	-33.742	-41.708	15.464	1.00	24.25
4563	O	LEU	B	96	-32.956	-41.799	16.401	1.00	22.95
4564	CB	LEU	B	96	-34.633	-39.435	14.916	1.00	20.55
4565	CG	LEU	B	96	-34.37	-38.034	14.347	1.00	20.54
4566	CD1	LEU	B	96	-35.573	-37.141	14.605	1.00	20.09
4567	CD2	LEU	B	96	-33.111	-37.441	14.975	1.00	17.62
4568	N	GLU	B	97	-34.701	-42.601	15.221	1.00	27.99
4569	CA	GLU	B	97	-34.918	-43.791	16.052	1.00	31.25
4570	C	GLU	B	97	-33.636	-44.611	16.216	1.00	32.02
4571	O	GLU	B	97	-33.309	-45.061	17.318	1.00	31.05
4572	CB	GLU	B	97	-36.02	-44.671	15.425	1.00	34.07
4573	CG	GLU	B	97	-35.778	-46.197	15.505	1.00	38.23
4574	CD	GLU	B	97	-36.07	-46.94	14.174	1.00	41.75
4575	OE1	GLU	B	97	-35.82	-48.175	14.094	1.00	41.45
4576	OE2	GLU	B	97	-36.548	-46.294	13.212	1.00	39.4
4577	N	GLU	B	98	-32.915	-44.794	15.115	1.00	32.5
4578	CA	GLU	B	98	-31.678	-45.573	15.114	1.00	34.37
4579	C	GLU	B	98	-30.514	-44.806	15.737	1.00	34.83
4580	O	GLU	B	98	-30.552	-43.582	15.854	1.00	35.91
4581	CB	GLU	B	98	-31.345	-45.984	13.673	1.00	34.6
4582	CG	GLU	B	98	-32.525	-46.669	12.97	1.00	36.04
4583	CD	GLU	B	98	-32.363	-46.796	11.459	1.00	37.49
4584	OE1	GLU	B	98	-31.859	-45.848	10.82	1.00	39.2
4585	OE2	GLU	B	98	-32.766	-47.839	10.904	1.00	38.91
4586	N	ALA	B	99	-29.484	-45.523	16.161	1.00	36.18
4587	CA	ALA	B	99	-28.323	-44.862	16.757	1.00	38.55
4588	C	ALA	B	99	-27.593	-44.11	15.644	1.00	38.88
4589	O	ALA	B	99	-27.439	-42.89	15.691	1.00	38.46
4590	CB	ALA	B	99	-27.391	-45.9	17.389	1.00	37.68
4591	N	LYS	B	100	-27.169	-44.885	14.647	1.00	38.22
4592	CA	LYS	B	100	-26.447	-44.44	13.458	1.00	36.88
4593	C	LYS	B	100	-26.279	-42.937	13.23	1.00	35.21
4594	O	LYS	B	100	-27.162	-42.14	13.524	1.00	35.52
4595	CB	LYS	B	100	-27.098	-45.079	12.22	1.00	37.02
4596	CG	LYS	B	100	-26.328	-44.88	10.923	1.00	37.83
4597	CD	LYS	B	100	-26.973	-45.629	9.761	1.00	38.69
4598	CE	LYS	B	100	-26.182	-45.401	8.477	1.00	40
4599	NZ	LYS	B	100	-26.764	-46.127	7.319	1.00	40.87

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TABLE 3

STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

4600	N	THR	B	101	-25.119	-42.565	12.701	1.00	32.81
4601	CA	THR	B	101	-24.818	-41.177	12.384	1.00	30.5
4602	C	THR	B	101	-25.225	-40.958	10.931	1.00	30.04
4603	O	THR	B	101	-24.78	-41.691	10.044	1.00	31.73
4604	CB	THR	B	101	-23.316	-40.886	12.508	1.00	29.39
4605	OG1	THR	B	101	-22.926	-40.947	13.883	1.00	27.21
4606	CG2	THR	B	101	-23	-39.507	11.948	1.00	31.25
4607	N	TYR	B	102	-26.074	-39.963	10.688	1.00	27.43
4608	CA	TYR	B	102	-26.534	-39.669	9.334	1.00	24.37
4609	C	TYR	B	102	-25.915	-38.395	8.778	1.00	21.53
4610	O	TYR	B	102	-25.724	-38.257	7.569	1.00	18.57
4611	CB	TYR	B	102	-28.062	-39.584	9.3	1.00	24.94
4612	CG	TYR	B	102	-28.7	-40.946	9.28	1.00	26.37
4613	CD1	TYR	B	102	-29.071	-41.587	10.467	1.00	27.22
4614	CD2	TYR	B	102	-28.864	-41.636	8.075	1.00	25.5
4615	CE1	TYR	B	102	-29.589	-42.888	10.453	1.00	27.19
4616	CE2	TYR	B	102	-29.376	-42.932	8.048	1.00	27.02
4617	CZ	TYR	B	102	-29.736	-43.554	9.237	1.00	28.15
4618	OH	TYR	B	102	-30.234	-44.841	9.207	1.00	29.32
4619	N	VAL	B	103	-25.616	-37.464	9.674	1.00	19.61
4620	CA	VAL	B	103	-24.979	-36.215	9.302	1.00	17.94
4621	C	VAL	B	103	-23.698	-36.183	10.108	1.00	18.73
4622	O	VAL	B	103	-23.706	-35.866	11.301	1.00	20.15
4623	CB	VAL	B	103	-25.846	-35.003	9.66	1.00	18.17
4624	CG1	VAL	B	103	-25.085	-33.722	9.35	1.00	16.3
4625	CG2	VAL	B	103	-27.158	-35.051	8.866	1.00	16.24
4626	N	ASN	B	104	-22.592	-36.528	9.459	1.00	17.87
4627	CA	ASN	B	104	-21.315	-36.577	10.146	1.00	17.93
4628	C	ASN	B	104	-20.728	-35.23	10.539	1.00	18.59
4629	O	ASN	B	104	-20.777	-34.265	9.774	1.00	17.18
4630	CB	ASN	B	104	-20.292	-37.333	9.307	1.00	17.5
4631	CG	ASN	B	104	-18.953	-37.428	9.997	1.00	18.51
4632	OD1	ASN	B	104	-18.852	-37.983	11.089	1.00	18.33
4633	ND2	ASN	B	104	-17.917	-36.874	9.372	1.00	18.59
4634	N	THR	B	105	-20.168	-35.179	11.742	1.00	18.56
4635	CA	THR	B	105	-19.533	-33.967	12.239	1.00	21.43
4636	C	THR	B	105	-18.175	-34.322	12.84	1.00	22.43
4637	O	THR	B	105	-17.466	-33.456	13.355	1.00	23.21
4638	CB	THR	B	105	-20.385	-33.27	13.316	1.00	21.96
4639	OG1	THR	B	105	-20.609	-34.171	14.405	1.00	25.8

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

4640	CG2	THR	B	105	-21.718	-32.831	12.744	1.00	22.45
4641	N	THR	B	106	-17.811	-35.6	12.764	1.00	22.74
4642	CA	THR	B	106	-16.54	-36.057	13.308	1.00	23.32
4643	C	THR	B	106	-15.454	-35.836	12.265	1.00	23.51
4644	O	THR	B	106	-15.654	-36.118	11.082	1.00	22.22
4645	CB	THR	B	106	-16.606	-37.548	13.689	1.00	24.42
4646	OG1	THR	B	106	-17.759	-37.774	14.505	1.00	25.81
4647	CG2	THR	B	106	-15.367	-37.951	14.469	1.00	23.26
4648	N	LEU	B	107	-14.304	-35.338	12.708	1.00	23.75
4649	CA	LEU	B	107	-13.199	-35.037	11.801	1.00	25.74
4650	C	LEU	B	107	-12.557	-36.215	11.054	1.00	27.87
4651	O	LEU	B	107	-12.3	-36.12	9.849	1.00	26.86
4652	CB	LEU	B	107	-12.11	-34.28	12.551	1.00	23.35
4653	CG	LEU	B	107	-12.484	-32.878	13.104	1.00	24.77
4654	CD1	LEU	B	107	-11.245	-32.233	13.726	1.00	24.39
4655	CD2	LEU	B	107	-13.044	-31.991	11.993	1.00	21.05
4656	N	TYR	B	108	-12.306	-37.315	11.763	1.00	29.48
4657	CA	TYR	B	108	-11.665	-38.483	11.173	1.00	30.81
4658	C	TYR	B	108	-10.373	-38.062	10.481	1.00	31.52
4659	O	TYR	B	108	-9.49	-37.479	11.108	1.00	31.73
4660	CB	TYR	B	108	-12.591	-39.179	10.171	1.00	32.42
4661	CG	TYR	B	108	-13.788	-39.844	10.805	1.00	34.73
4662	CD1	TYR	B	108	-15.07	-39.327	10.633	1.00	35.15
4663	CD2	TYR	B	108	-13.64	-40.993	11.587	1.00	36.52
4664	CE1	TYR	B	108	-16.177	-39.936	11.22	1.00	35.82
4665	CE2	TYR	B	108	-14.743	-41.611	12.183	1.00	35.88
4666	CZ	TYR	B	108	-16.006	-41.074	11.992	1.00	36.31
4667	OH	TYR	B	108	-17.097	-41.67	12.572	1.00	37.43
4668	N	GLU	B	109	-10.256	-38.345	9.19	1.00	31.72
4669	CA	GLU	B	109	-9.045	-37.981	8.477	1.00	33.92
4670	C	GLU	B	109	-9.198	-36.804	7.529	1.00	32.27
4671	O	GLU	B	109	-8.219	-36.342	6.946	1.00	31.36
4672	CB	GLU	B	109	-8.505	-39.188	7.712	1.00	38.74
4673	CG	GLU	B	109	-7.964	-40.278	8.625	1.00	45.06
4674	CD	GLU	B	109	-6.853	-41.071	7.976	1.00	48.93
4675	OE1	GLU	B	109	-6.278	-41.953	8.651	1.00	52.43
4676	OE2	GLU	B	109	-6.551	-40.809	6.79	1.00	51.3
4677	N	LYS	B	110	-10.417	-36.301	7.39	1.00	30.21
4678	CA	LYS	B	110	-10.643	-35.189	6.487	1.00	28.89
4679	C	LYS	B	110	-12.073	-34.662	6.564	1.00	26.97



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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

4680	O	LYS	B	110	-13.031	-35.426	6.465	1.00	27.5
4681	CB	LYS	B	110	-10.327	-35.645	5.062	1.00	29.78
4682	CG	LYS	B	110	-10.484	-34.597	3.987	1.00	33.42
4683	CD	LYS	B	110	-10.221	-35.223	2.621	1.00	35.61
4684	CE	LYS	B	110	-10.446	-34.237	1.489	1.00	37.59
4685	NZ	LYS	B	110	-10.228	-34.883	0.159	1.00	40.37
4686	N	PHE	B	111	-12.215	-33.357	6.759	1.00	24.36
4687	CA	PHE	B	111	-13.535	-32.751	6.807	1.00	22.17
4688	C	PHE	B	111	-13.518	-31.441	6.041	1.00	19.91
4689	O	PHE	B	111	-12.6	-30.634	6.178	1.00	16.83
4690	CB	PHE	B	111	-13.992	-32.514	8.245	1.00	21.77
4691	CG	PHE	B	111	-15.438	-32.112	8.352	1.00	24.09
4692	CD1	PHE	B	111	-15.841	-30.81	8.058	1.00	23.12
4693	CD2	PHE	B	111	-16.406	-33.046	8.709	1.00	23.65
4694	CE1	PHE	B	111	-17.181	-30.448	8.116	1.00	23.37
4695	CE2	PHE	B	111	-17.753	-32.689	8.77	1.00	23.87
4696	CZ	PHE	B	111	-18.139	-31.387	8.472	1.00	22.59
4697	N	THR	B	112	-14.547	-31.236	5.23	1.00	19.4
4698	CA	THR	B	112	-14.635	-30.037	4.415	1.00	17.96
4699	C	THR	B	112	-15.877	-29.211	4.727	1.00	16.84
4700	O	THR	B	112	-16.982	-29.739	4.794	1.00	17.4
4701	CB	THR	B	112	-14.633	-30.419	2.923	1.00	18.55
4702	OG1	THR	B	112	-13.468	-31.211	2.644	1.00	17.92
4703	CG2	THR	B	112	-14.616	-29.161	2.042	1.00	17.73
4704	N	TYR	B	113	-15.679	-27.913	4.931	1.00	15.98
4705	CA	TYR	B	113	-16.778	-26.994	5.216	1.00	15.63
4706	C	TYR	B	113	-17.328	-26.448	3.897	1.00	16.81
4707	O	TYR	B	113	-16.574	-25.929	3.067	1.00	16.84
4708	CB	TYR	B	113	-16.292	-25.818	6.07	1.00	14.65
4709	CG	TYR	B	113	-16.297	-26.032	7.571	1.00	15.57
4710	CD1	TYR	B	113	-15.535	-25.213	8.402	1.00	17.47
4711	CD2	TYR	B	113	-17.068	-27.03	8.166	1.00	14.9
4712	CE1	TYR	B	113	-15.531	-25.377	9.783	1.00	16.04
4713	CE2	TYR	B	113	-17.071	-27.205	9.554	1.00	13.34
4714	CZ	TYR	B	113	-16.295	-26.373	10.349	1.00	15.94
4715	OH	TYR	B	113	-16.25	-26.542	11.711	1.00	18.09
4716	N	ALA	B	114	-18.638	-26.568	3.701	1.00	17.32
4717	CA	ALA	B	114	-19.275	-26.065	2.489	1.00	16.9
4718	C	ALA	B	114	-19.033	-24.563	2.414	1.00	17.72
4719	O	ALA	B	114	-18.936	-23.883	3.445	1.00	15.35

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

4720	CB	ALA	B	114	-20.779	-26.354	2.517	1.00	15.9
4721	N	GLY	B	115	-18.951	-24.053	1.189	1.00	18.38
4722	CA	GLY	B	115	-18.712	-22.638	0.985	1.00	21.57
4723	C	GLY	B	115	-19.839	-21.683	1.341	1.00	24.3
4724	O	GLY	B	115	-21.029	-22.017	1.297	1.00	22.45
4725	N	ILE	B	116	-19.438	-20.472	1.703	1.00	27.87
4726	CA	ILE	B	116	-20.362	-19.408	2.056	1.00	31.94
4727	C	ILE	B	116	-19.957	-18.19	1.228	1.00	35.86
4728	O	ILE	B	116	-19.109	-17.392	1.634	1.00	35.25
4729	CB	ILE	B	116	-20.281	-19.083	3.564	1.00	30.12
4730	CG1	ILE	B	116	-20.762	-20.287	4.372	1.00	28.71
4731	CG2	ILE	B	116	-21.131	-17.863	3.89	1.00	31.16
4732	CD1	ILE	B	116	-20.557	-20.144	5.87	1.00	27.47
4733	N	ASP	B	117	-20.547	-18.085	0.042	1.00	42.11
4734	CA	ASP	B	117	-20.275	-16.984	-0.876	1.00	48
4735	C	ASP	B	117	-21.206	-15.84	-0.516	1.00	51.35
4736	O	ASP	B	117	-22.352	-15.801	-0.965	1.00	51.75
4737	CB	ASP	B	117	-20.526	-17.434	-2.322	1.00	49.82
4738	CG	ASP	B	117	-20.319	-16.313	-3.34	1.00	52.67
4739	OD1	ASP	B	117	-19.2	-15.753	-3.411	1.00	53.87
4740	OD2	ASP	B	117	-21.278	-16	-4.079	1.00	53.29
4741	N	CYS	B	118	-20.715	-14.92	0.311	1.00	54.64
4742	CA	CYS	B	118	-21.508	-13.773	0.74	1.00	58.27
4743	C	CYS	B	118	-21.766	-12.811	-0.424	1.00	59.32
4744	O	CYS	B	118	-22.305	-11.718	-0.229	1.00	59.43
4745	CB	CYS	B	118	-20.797	-13.032	1.885	1.00	60.53
4746	SG	CYS	B	118	-20.598	-13.981	3.436	1.00	64.6
4747	N	ALA	B	119	-21.376	-13.227	-1.629	1.00	60.12
4748	CA	ALA	B	119	-21.567	-12.425	-2.838	1.00	60.91
4749	C	ALA	B	119	-22.97	-12.665	-3.396	1.00	61.23
4750	O	ALA	B	119	-23.376	-12.062	-4.394	1.00	60.87
4751	CB	ALA	B	119	-20.509	-12.792	-3.887	1.00	60.98
4752	N	ALA	B	120	-23.7	-13.562	-2.739	1.00	61.53
4753	CA	ALA	B	120	-25.064	-13.9	-3.124	1.00	61.6
4754	C	ALA	B	120	-25.97	-13.703	-1.911	1.00	61.56
4755	O	ALA	B	120	-27.108	-14.17	-1.892	1.00	62.09
4756	CB	ALA	B	120	-25.13	-15.347	-3.604	1.00	60.65
4757	N	GLU	B	121	-25.451	-13.003	-0.903	1.00	61.65
4758	CA	GLU	B	121	-26.187	-12.733	0.331	1.00	61.81
4759	C	GLU	B	121	-26.18	-11.246	0.69	1.00	62.1

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

4760	O	GLU	B	121	-25.413	-10.865	1.599	1.00	62.54
4761	CB	GLU	B	121	-25.589	-13.545	1.485	1.00	61.2
4762	CG	GLU	B	121	-25.618	-15.05	1.254	1.00	61.01
4763	CD	GLU	B	121	-25.076	-15.839	2.431	1.00	59.98
4764	OE1	GLU	B	121	-25.639	-15.723	3.542	1.00	59.44
4765	OE2	GLU	B	121	-24.089	-16.576	2.241	1.00	59.17
4766	OXT	GLU	B	121	-26.933	-10.475	0.053	1.00	62.19
4767	O	HOH		1	-42.862	1.859	27.005	1.00	19.47
4768	O	HOH		2	-45.505	6.474	12.991	1.00	25.87
4769	O	HOH		3	-44.352	10.19	14.853	1.00	24.34
4770	O	HOH		4	-46.007	6.685	16.239	1.00	40.56
4771	O	HOH		5	-44.542	12.043	17.664	1.00	48.35
4772	O	HOH		6	-38.775	13.359	18.624	1.00	26.64
4773	O	HOH		7	-45.973	14.598	14.895	1.00	25.79
4774	O	HOH		8	-41.671	13.129	11.78	1.00	8.71
4775	O	HOH		9	-42.541	14.143	8.908	1.00	25.29
4776	O	HOH		10	-39.912	11.019	9.74	1.00	30.15
4777	O	HOH		11	-39.209	13.522	6.434	1.00	23.19
4778	O	HOH		12	-33.808	8.4	7.254	1.00	29.13
4779	O	HOH		13	-33.209	15.782	4.001	1.00	25.04
4780	O	HOH		14	-35.568	14.339	3.698	1.00	39.94
4781	O	HOH		15	-34.005	15.524	23.917	1.00	17.52
4782	O	HOH		16	-36.534	17.096	24.839	1.00	34.58
4783	O	HOH		17	-42.113	11.985	27.747	1.00	28.91
4784	O	HOH		18	-25.333	12.519	5.714	1.00	21.5
4785	O	HOH		19	-26.663	15.191	8.141	1.00	24.56
4786	O	HOH		20	-25.874	12.216	8.289	1.00	24.07
4787	O	HOH		21	-21.954	15.367	1.896	1.00	15.55
4788	O	HOH		22	-22.047	17.406	15.793	1.00	23.62
4789	O	HOH		23	-29.583	-7.064	13.725	1.00	31.67
4790	O	HOH		24	-36.553	19.419	22.039	1.00	16.48
4791	O	HOH		25	-34.449	20.094	23.507	1.00	17.57
4792	O	HOH		26	-42.612	22.233	25.441	1.00	23.26
4793	O	HOH		27	-47.799	18.816	24.488	1.00	29.32
4794	O	HOH		28	-48.185	19.143	21.614	1.00	18.2
4795	O	HOH		29	-48.381	17.645	16.824	1.00	44.73
4796	O	HOH		30	-47.736	14.567	10.014	1.00	33.69
4797	O	HOH		31	-45.636	14.323	8.058	1.00	32.37
4798	O	HOH		32	-45.859	14.664	5.191	1.00	23.88
4799	O	HOH		33	-43.892	19.412	4.796	1.00	11.48

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TABLE 3

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

4800	O	HOH		34	-51.239	22.393	17.356	1.00	19.16
4801	O	HOH		35	-52.458	36.883	15.631	1.00	30.59
4802	O	HOH		36	-49.57	37.901	16.905	1.00	28.78
4803	O	HOH		37	-49.492	40.259	15.698	1.00	21.64
4804	O	HOH		38	-50.045	37.831	19.654	1.00	36.39
4805	O	HOH		39	-51.381	31.655	20.381	1.00	29.94
4806	O	HOH		40	-44.803	34.683	20.289	1.00	26.79
4807	O	HOH		41	-39.396	31.542	19.251	1.00	26.06
4808	O	HOH		42	-37.49	30.111	19.065	1.00	34.85
4809	O	HOH		43	-40.792	29.436	18.549	1.00	20.43
4810	O	HOH		44	-43.383	30.269	17.587	1.00	23.91
4811	O	HOH		45	-44.193	30.382	21.24	1.00	30.36
4812	O	HOH		46	-43.367	32.094	19.568	1.00	35.68
4813	O	HOH		47	-41.119	31.57	25.676	1.00	58.73
4814	O	HOH		48	-32.537	36.154	15.351	1.00	28.55
4815	O	HOH		49	-27.764	25.561	2.669	1.00	10.93
4816	O	HOH		50	-24.334	25.59	2.296	1.00	17.16
4817	O	HOH		51	-22.82	25.293	0.258	1.00	17.39
4818	O	HOH		52	-24.386	25.774	-2.118	1.00	27.04
4819	O	HOH		53	-34.253	22.12	0.54	1.00	13.1
4820	O	HOH		54	-32.126	22.191	-2.035	1.00	16.3
4821	O	HOH		55	-31.951	14.545	-1.938	1.00	19.24
4822	O	HOH		56	-38.347	19.108	0.174	1.00	24.69
4823	O	HOH		57	-34.29	21.656	28.479	1.00	25.21
4824	O	HOH		58	-41.364	22.768	-7.346	1.00	10.72
4825	O	HOH		59	-42.027	24.804	-5.466	1.00	22.43
4826	O	HOH		60	-34.951	21.785	-4.505	1.00	23.1
4827	O	HOH		61	-33.196	14.322	-6.868	1.00	35.66
4828	O	HOH		62	-26.675	28.29	-7.217	1.00	20.37
4829	O	HOH		63	-28.66	26.588	-7.292	1.00	30
4830	O	HOH		64	-25.132	32.24	-4.88	1.00	28.91
4831	O	HOH		65	-47.857	21.212	3.236	1.00	12.3
4832	O	HOH		66	-55.251	27.856	5.608	1.00	17.83
4833	O	HOH		67	-54.022	30.316	4.353	1.00	20.08
4834	O	HOH		68	-56.971	32.185	4.561	1.00	30.37
4835	O	HOH		69	-54.931	30.135	1.385	1.00	26.31
4836	O	HOH		70	-53.11	24.134	-0.001	1.00	16.26
4837	O	HOH		71	-52.233	25.897	-3.611	1.00	27.11
4838	O	HOH		72	-56.789	25.417	-1.368	1.00	22.96
4839	O	HOH		73	-38.864	30.999	-13.758	1.00	34.99

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

4840	O	HOH		74	-41.338	34.1	-7.967	1.00	18.61
4841	O	HOH		75	-43.742	28.734	-6.211	1.00	9.19
4842	O	HOH		76	-52.21	28.803	-5.728	1.00	31.83
4843	O	HOH		77	-60.926	33.932	3.423	1.00	23.99
4844	O	HOH		78	-58.121	36.161	6.361	1.00	25.91
4845	O	HOH		79	-51.008	42.95	2.594	1.00	21.56
4846	O	HOH		80	-55.655	40.128	12.853	1.00	32.74
4847	O	HOH		81	-43.059	49.818	11.299	1.00	61.07
4848	O	HOH		82	-41.859	49.023	16.121	1.00	43.18
4849	O	HOH		83	-45.473	41.475	13.89	1.00	25.14
4850	O	HOH		84	-32.545	41.45	4.328	1.00	23.92
4851	O	HOH		85	-26.865	33.277	5.586	1.00	13.41
4852	O	HOH		86	-24.952	35.462	4.963	1.00	33.56
4853	O	HOH		87	-26.307	37.572	3.61	1.00	27.16
4854	O	HOH		88	-24.81	38.079	0.675	1.00	31.72
4855	O	HOH		89	-26.9	34.705	-1.325	1.00	28.83
4856	O	HOH		90	-27.441	37.047	-1.331	1.00	29.7
4857	O	HOH		91	-30.887	39.866	-2.432	1.00	34.61
4858	O	HOH		92	-33.353	40.587	-1.086	1.00	26.38
4859	O	HOH		93	-34.699	35.728	-11.326	1.00	21.63
4860	O	HOH		94	-37.758	35.363	-11.334	1.00	26.52
4861	O	HOH		95	-51.021	-6.703	28.928	1.00	24.57
4862	O	HOH		96	-53.153	-0.387	26.089	1.00	26.87
4863	O	HOH		97	-33.555	-13.16	11.659	1.00	14.65
4864	O	HOH		98	-33.002	-14.181	9.016	1.00	16.96
4865	O	HOH		99	-36.095	-13.389	6.257	1.00	18.87
4866	O	HOH		100	-39.526	-13.927	3.389	1.00	24.33
4867	O	HOH		101	-42.119	-15.632	4.021	1.00	26.34
4868	O	HOH		102	-40.668	-3.632	14.526	1.00	22.79
4869	O	HOH		103	-42.672	-3.148	10.624	1.00	40.71
4870	O	HOH		104	-38.371	-14.423	34.161	1.00	52.27
4871	O	HOH		105	-34.399	-9.783	30.135	1.00	44.16
4872	O	HOH		106	-41.347	-15.709	24.037	1.00	16.16
4873	O	HOH		107	-33.673	-17.05	24.865	1.00	25.15
4874	O	HOH		108	-48.547	-14.891	7.713	1.00	27.22
4875	O	HOH		109	-53.544	-17.916	15.705	1.00	22.67
4876	O	HOH		110	-54.467	-24.645	17.459	1.00	23.31
4877	O	HOH		111	-42.534	-25.022	22.17	1.00	40.55
4878	O	HOH		112	-39.659	-24.907	23.744	1.00	27.96
4879	O	HOH		113	-36.35	-13.602	18.724	1.00	19.76

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

4880	O	HOH		114	-38.509	-19.675	21.769	1.00	18.89
4881	O	HOH		115	-23.27	-16.594	11.197	1.00	41.97
4882	O	HOH		116	-24.156	-22.281	17.063	1.00	15.82
4883	O	HOH		117	-24.35	-19.898	18.777	1.00	28.79
4884	O	HOH		118	-23.847	-23.843	19.293	1.00	31.18
4885	O	HOH		119	-19.693	-19.37	17.897	1.00	33.09
4886	O	HOH		120	-11.396	-36.312	20.63	1.00	23.59
4887	O	HOH		121	-19.159	-31.965	19.863	1.00	34.75
4888	O	HOH		122	-24.033	-31.95	21.349	1.00	35.68
4889	O	HOH		123	-24.62	-28.014	21.278	1.00	30.78
4890	O	HOH		124	-27.837	-39.168	13.763	1.00	22.49
4891	O	HOH		125	-26.467	-40.352	16.301	1.00	26.26
4892	O	HOH		126	-25.769	-37.945	17.16	1.00	29.11
4893	O	HOH		127	-22.669	-36.678	15.92	1.00	27.69
4894	O	HOH		128	-30.645	-29.837	22.006	1.00	25.99
4895	O	HOH		129	-30.599	-34.593	20.147	1.00	28.79
4896	O	HOH		130	-32.282	-31.761	19.936	1.00	19.19
4897	O	HOH		131	-31.826	-29.949	17.839	1.00	13.83
4898	O	HOH		132	-33.655	-38.344	19.669	1.00	34.94
4899	O	HOH		133	-35.433	-30.543	20.319	1.00	34.61
4900	O	HOH		134	-37.318	-33.047	16.635	1.00	28.42
4901	O	HOH		135	-42.736	-36.426	15.297	1.00	24.51
4902	O	HOH		136	-47.534	-32.024	12.349	1.00	15.47
4903	O	HOH		137	-48.25	-33.452	5.346	1.00	14.73
4904	O	HOH		138	-50.343	-35.274	4.837	1.00	28.72
4905	O	HOH		139	-51.57	-31.067	11.388	1.00	24.75
4906	O	HOH		140	-50.153	-34.754	13.22	1.00	34.99
4907	O	HOH		141	-48.169	-35.908	10.497	1.00	16.88
4908	O	HOH		142	-45.689	-38.086	9.649	1.00	19.89
4909	O	HOH		143	-52.278	-25.303	0.44	1.00	19.52
4910	O	HOH		144	-50.764	-25.702	-2.121	1.00	19.91
4911	O	HOH		145	-47.315	-25.313	2.649	1.00	10.25
4912	O	HOH		146	-43.061	-14.429	-2.48	1.00	19.48
4913	O	HOH		147	-36.402	-18.974	0.694	1.00	26.06
4914	O	HOH		148	-31.156	-19.341	4.72	1.00	10.32
4915	O	HOH		149	-27.342	-20.957	2.99	1.00	11.12
4916	O	HOH		150	-30.032	-17.112	3.58	1.00	22.6
4917	O	HOH		151	-29.481	-14.91	5.193	1.00	19.86
4918	O	HOH		152	-41.775	-28.657	21.542	1.00	22.13
4919	O	HOH		153	-49.745	-12.258	5.089	1.00	27.73

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TABLE 3  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM II

4920	O	HOH		154	-34.004	-22.888	-7.103	1.00	12.24
4921	O	HOH		155	-33.001	-24.782	-5.447	1.00	25.34
4922	O	HOH		156	-40.755	-21.932	-4.381	1.00	18.1
4923	O	HOH		157	-43.074	-21.904	-2.204	1.00	19.34
4924	O	HOH		158	-40.852	-21.746	0.466	1.00	8.82
4925	O	HOH		159	-42.547	-15.191	-7.53	1.00	37.65
4926	O	HOH		160	-46.704	-26.596	-7.586	1.00	18.47
4927	O	HOH		161	-48.493	-28.309	-7.415	1.00	21.69
4928	O	HOH		162	-21.179	-30.298	5.018	1.00	23.85
4929	O	HOH		163	-19.918	-27.816	5.651	1.00	11.98
4930	O	HOH		164	-20.13	-30.754	1.455	1.00	36.85
4931	O	HOH		165	-21.216	-26.397	-1.609	1.00	25.17
4932	O	HOH		166	-22.011	-24.165	-0.034	1.00	21.87
4933	O	HOH		167	-18.574	-25.285	-1.27	1.00	22.61
4934	O	HOH		168	-23.759	-26.544	-7.053	1.00	28.91
4935	O	HOH		169	-22.988	-28.318	-4.561	1.00	28.72
4936	O	HOH		170	-27.117	-14.5	-12.601	1.00	38.76
4937	O	HOH		171	-33.828	-34.317	-7.356	1.00	16.16
4938	O	HOH		172	-14.35	-33.977	3.432	1.00	19.39
4939	O	HOH		173	-16.553	-33.449	5.226	1.00	23.21
4940	O	HOH		174	-17.172	-36.016	6.751	1.00	15.76
4941	O	HOH		175	-24.13	-43.107	2.782	1.00	25.7
4942	O	HOH		176	-25.953	-46.907	4.835	1.00	32.42
4943	O	HOH		177	-27.618	-45.183	4.334	1.00	33.3
4944	O	HOH		178	-40.418	-39.487	2.489	1.00	20.25
4945	O	HOH		179	-41.575	-40.409	-1.371	1.00	32.75
4946	O	HOH		180	-36.618	-39.665	-6.374	1.00	28.55
4947	O	HOH		181	-40.576	-35.728	-11.182	1.00	17.21
4948	O	HOH		182	-37.297	-35.478	-11.142	1.00	25.65
4949	O	HOH		183	-50.202	-32.38	-4.869	1.00	31.32
4950	O	HOH		184	-47.374	-39.951	8.512	1.00	22.74
4951	O	HOH		185	-44.467	-39.229	11.903	1.00	25.99
4952	O	HOH		186	-41.096	-43.063	12.192	1.00	37.31
4953	O	HOH		187	-19.5	-40.207	12.779	1.00	28.16
4954	O	HOH		188	-14.624	-36.321	8.565	1.00	20.78

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TABLE 4

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

ATOM	ATOM TYPE	RESIDUE	PROTEIN #	#	X	Y	Z	OCC	B
1	N	ILE	A	815	21.536	16.204	25.781	1.00	46.01
2	CA	ILE	A	815	22.033	14.864	26.213	1.00	45.81
3	C	ILE	A	815	22.681	14.917	27.594	1.00	45.5
4	O	ILE	A	815	23.875	14.654	27.742	1.00	45.63
5	CB	ILE	A	815	23.065	14.298	25.209	1.00	45.99
6	CG1	ILE	A	815	24.127	15.359	24.903	1.00	46.12
7	CG2	ILE	A	815	22.358	13.826	23.944	1.00	46.14
8	CD1	ILE	A	815	25.266	14.864	24.029	1.00	46.34
9	N	TYR	A	816	21.886	15.257	28.605	1.00	44.99
10	CA	TYR	A	816	22.387	15.336	29.973	1.00	44.2
11	C	TYR	A	816	21.836	14.182	30.808	1.00	43.15
12	O	TYR	A	816	20.73	13.699	30.566	1.00	43.22
13	CB	TYR	A	816	21.994	16.675	30.609	1.00	45.1
14	CG	TYR	A	816	22.473	17.886	29.834	1.00	45.85
15	CD1	TYR	A	816	21.919	18.209	28.594	1.00	46.16
16	CD2	TYR	A	816	23.5	18.693	30.327	1.00	46.23
17	CE1	TYR	A	816	22.376	19.303	27.86	1.00	46.42
18	CE2	TYR	A	816	23.965	19.792	29.601	1.00	46.6
19	CZ	TYR	A	816	23.399	20.088	28.367	1.00	46.62
20	OH	TYR	A	816	23.863	21.159	27.634	1.00	46.91
21	N	PRO	A	817	22.608	13.723	31.804	1.00	41.9
22	CA	PRO	A	817	23.929	14.263	32.126	1.00	40.86
23	C	PRO	A	817	24.998	13.782	31.153	1.00	39.73
24	O	PRO	A	817	24.807	12.803	30.431	1.00	39.47
25	CB	PRO	A	817	24.168	13.75	33.54	1.00	41.14
26	CG	PRO	A	817	23.527	12.4	33.491	1.00	41.39
27	CD	PRO	A	817	22.216	12.691	32.78	1.00	41.71
28	N	VAL	A	818	26.119	14.49	31.131	1.00	38.42
29	CA	VAL	A	818	27.224	14.119	30.267	1.00	37.07
30	C	VAL	A	818	28.033	13.059	31.012	1.00	36.13
31	O	VAL	A	818	28.298	13.196	32.207	1.00	36
32	CB	VAL	A	818	28.131	15.333	29.961	1.00	37.2
33	CG1	VAL	A	818	29.265	14.917	29.033	1.00	36.87
34	CG2	VAL	A	818	27.31	16.452	29.332	1.00	36.91
35	N	LEU	A	819	28.402	11.995	30.308	1.00	34.86
36	CA	LEU	A	819	29.182	10.922	30.907	1.00	33.61
37	C	LEU	A	819	30.632	10.984	30.439	1.00	32.94
38	O	LEU	A	819	30.911	11.225	29.262	1.00	32.65
39	CB	LEU	A	819	28.582	9.555	30.547	1.00	33.35



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TABLE 4  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

40	CG	LEU	A	819	27.207	9.197	31.123	1.00	33.24
41	CD1	LEU	A	819	26.808	7.815	30.643	1.00	33.08
42	CD2	LEU	A	819	27.246	9.238	32.652	1.00	32.99
43	N	ASP	A	820	31.555	10.776	31.371	1.00	32.28
44	CA	ASP	A	820	32.975	10.795	31.05	1.00	31.66
45	C	ASP	A	820	33.322	9.466	30.392	1.00	30.81
46	O	ASP	A	820	33.003	8.403	30.93	1.00	30.34
47	CB	ASP	A	820	33.81	10.956	32.321	1.00	32.4
48	CG	ASP	A	820	35.293	11.108	32.03	1.00	33.31
49	OD1	ASP	A	820	35.75	10.649	30.956	1.00	33.81
50	OD2	ASP	A	820	36.01	11.675	32.883	1.00	34.09
51	N	TRP	A	821	33.971	9.529	29.233	1.00	29.82
52	CA	TRP	A	821	34.36	8.321	28.521	1.00	29.24
53	C	TRP	A	821	35.19	7.406	29.41	1.00	28.95
54	O	TRP	A	821	35.027	6.191	29.378	1.00	28.76
55	CB	TRP	A	821	35.148	8.673	27.249	1.00	28.67
56	CG	TRP	A	821	35.802	7.485	26.604	1.00	28.22
57	CD1	TRP	A	821	37.088	7.056	26.785	1.00	28.12
58	CD2	TRP	A	821	35.184	6.531	25.729	1.00	28.09
59	NE1	TRP	A	821	37.307	5.896	26.082	1.00	27.88
60	CE2	TRP	A	821	36.156	5.551	25.425	1.00	28
61	CE3	TRP	A	821	33.902	6.407	25.174	1.00	28.08
62	CZ2	TRP	A	821	35.886	4.459	24.589	1.00	27.92
63	CZ3	TRP	A	821	33.634	5.319	24.342	1.00	27.94
64	CH2	TRP	A	821	34.623	4.362	24.059	1.00	27.94
65	N	ASN	A	822	36.066	7.995	30.217	1.00	29.17
66	CA	ASN	A	822	36.928	7.217	31.101	1.00	29.53
67	C	ASN	A	822	36.183	6.429	32.184	1.00	29.35
68	O	ASN	A	822	36.707	5.443	32.702	1.00	29.63
69	CB	ASN	A	822	37.979	8.124	31.756	1.00	30.3
70	CG	ASN	A	822	38.878	8.816	30.734	1.00	30.97
71	OD1	ASN	A	822	39.095	8.307	29.633	1.00	31.52
72	ND2	ASN	A	822	39.421	9.97	31.106	1.00	31.4
73	N	ASP	A	823	34.967	6.854	32.52	1.00	29.01
74	CA	ASP	A	823	34.182	6.164	33.542	1.00	28.82
75	C	ASP	A	823	33.308	5.053	32.97	1.00	28.31
76	O	ASP	A	823	32.468	4.488	33.674	1.00	28.6
77	CB	ASP	A	823	33.279	7.148	34.3	1.00	29.25
78	CG	ASP	A	823	34.062	8.108	35.175	1.00	29.94
79	OD1	ASP	A	823	35.094	7.685	35.739	1.00	29.92

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TABLE 4  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

80	OD2	ASP	A	823	33.631	9.279	35.311	1.00	30.4
81	N	ILE	A	824	33.497	4.733	31.697	1.00	27.41
82	CA	ILE	A	824	32.694	3.69	31.081	1.00	26.42
83	C	ILE	A	824	33.507	2.426	30.827	1.00	26.16
84	O	ILE	A	824	34.566	2.472	30.204	1.00	26.06
85	CB	ILE	A	824	32.091	4.184	29.752	1.00	26.1
86	CG1	ILE	A	824	31.316	5.481	29.991	1.00	25.78
87	CG2	ILE	A	824	31.187	3.119	29.162	1.00	25.67
88	CD1	ILE	A	824	30.712	6.088	28.739	1.00	25.48
89	N	LYS	A	825	33.015	1.301	31.335	1.00	25.69
90	CA	LYS	A	825	33.681	0.024	31.138	1.00	25.41
91	C	LYS	A	825	32.71	-0.868	30.376	1.00	25.15
92	O	LYS	A	825	31.682	-1.278	30.911	1.00	24.94
93	CB	LYS	A	825	34.04	-0.624	32.483	1.00	25.83
94	CG	LYS	A	825	34.766	0.295	33.466	1.00	26.33
95	CD	LYS	A	825	36.066	0.89	32.909	1.00	26.67
96	CE	LYS	A	825	37.18	-0.135	32.82	1.00	26.85
97	NZ	LYS	A	825	38.521	0.503	32.601	1.00	27.03
98	N	PHE	A	826	33.037	-1.161	29.123	1.00	24.81
99	CA	PHE	A	826	32.183	-1.993	28.289	1.00	24.85
100	C	PHE	A	826	32.364	-3.48	28.55	1.00	25.4
101	O	PHE	A	826	33.423	-3.925	28.993	1.00	25.2
102	CB	PHE	A	826	32.451	-1.72	26.806	1.00	24.11
103	CG	PHE	A	826	32.256	-0.292	26.405	1.00	23.39
104	CD1	PHE	A	826	33.293	0.623	26.518	1.00	23.36
105	CD2	PHE	A	826	31.032	0.14	25.902	1.00	23.06
106	CE1	PHE	A	826	33.115	1.96	26.13	1.00	23.35
107	CE2	PHE	A	826	30.846	1.468	25.513	1.00	22.88
108	CZ	PHE	A	826	31.89	2.377	25.627	1.00	22.77
109	N	GLN	A	827	31.318	-4.243	28.258	1.00	26.11
110	CA	GLN	A	827	31.343	-5.685	28.433	1.00	27.19
111	C	GLN	A	827	30.775	-6.338	27.176	1.00	27.74
112	O	GLN	A	827	31.056	-5.885	26.067	1.00	27.97
113	CB	GLN	A	827	30.542	-6.071	29.675	1.00	27.64
114	CG	GLN	A	827	30.963	-5.276	30.902	1.00	28.58
115	CD	GLN	A	827	30.169	-5.621	32.145	1.00	29.16
116	OE1	GLN	A	827	30.336	-6.694	32.721	1.00	29.99
117	NE2	GLN	A	827	29.299	-4.708	32.567	1.00	29.15
118	N	ASP	A	828	29.969	-7.381	27.339	1.00	28.45
119	CA	ASP	A	828	29.402	-8.095	26.197	1.00	29

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

120	C	ASP	A	828	28.194	-7.438	25.529	1.00	28.81
121	O	ASP	A	828	27.51	-6.605	26.121	1.00	28.69
122	CB	ASP	A	828	29.033	-9.52	26.616	1.00	30.08
123	CG	ASP	A	828	30.243	-10.33	27.042	1.00	31.5
124	OD1	ASP	A	828	31.18	-10.477	26.216	1.00	32.27
125	OD2	ASP	A	828	30.26	-10.816	28.199	1.00	31.85
126	N	VAL	A	829	27.942	-7.837	24.284	1.00	28.36
127	CA	VAL	A	829	26.821	-7.32	23.511	1.00	27.93
128	C	VAL	A	829	25.548	-8.05	23.915	1.00	27.51
129	O	VAL	A	829	25.588	-9.219	24.292	1.00	27.61
130	CB	VAL	A	829	27.041	-7.522	21.993	1.00	28.11
131	CG1	VAL	A	829	25.848	-6.979	21.211	1.00	27.95
132	CG2	VAL	A	829	28.32	-6.821	21.557	1.00	28.17
133	N	ILE	A	830	24.421	-7.35	23.837	1.00	26.91
134	CA	ILE	A	830	23.126	-7.919	24.189	1.00	26.07
135	C	ILE	A	830	22.014	-7.206	23.425	1.00	25.77
136	O	ILE	A	830	22.243	-6.177	22.78	1.00	25.53
137	CB	ILE	A	830	22.818	-7.761	25.694	1.00	26.19
138	CG1	ILE	A	830	22.723	-6.271	26.048	1.00	25.79
139	CG2	ILE	A	830	23.88	-8.468	26.535	1.00	25.83
140	CD1	ILE	A	830	22.256	-6.011	27.463	1.00	25.8
141	N	GLY	A	831	20.806	-7.756	23.511	1.00	25.25
142	CA	GLY	A	831	19.669	-7.155	22.842	1.00	24.81
143	C	GLY	A	831	18.77	-6.472	23.854	1.00	24.43
144	O	GLY	A	831	18.563	-6.986	24.961	1.00	24.53
145	N	GLU	A	832	18.243	-5.307	23.495	1.00	23.82
146	CA	GLU	A	832	17.358	-4.6	24.4	1.00	23.27
147	C	GLU	A	832	16.165	-4.011	23.665	1.00	22.72
148	O	GLU	A	832	16.09	-2.803	23.449	1.00	22.23
149	CB	GLU	A	832	18.112	-3.498	25.152	1.00	23.45
150	CG	GLU	A	832	17.373	-3.028	26.401	1.00	23.84
151	CD	GLU	A	832	18.263	-2.287	27.377	1.00	24.12
152	OE1	GLU	A	832	19.444	-2.665	27.508	1.00	24.79
153	OE2	GLU	A	832	17.779	-1.341	28.032	1.00	24.27
154	N	GLY	A	833	15.232	-4.881	23.281	1.00	22.26
155	CA	GLY	A	833	14.039	-4.433	22.584	1.00	21.76
156	C	GLY	A	833	14.341	-3.612	21.346	1.00	21.83
157	O	GLY	A	833	15.305	-3.889	20.623	1.00	21.68
158	N	ASN	A	834	13.529	-2.591	21.096	1.00	21.65
159	CA	ASN	A	834	13.741	-1.772	19.917	1.00	21.79

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## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

160	C	ASN	A	834	15.041	-0.955	19.92	1.00	22.14
161	O	ASN	A	834	15.29	-0.187	18.992	1.00	22.2
162	CB	ASN	A	834	12.524	-0.869	19.646	1.00	20.91
163	CG	ASN	A	834	12.065	-0.101	20.868	1.00	20.61
164	OD1	ASN	A	834	12.863	0.259	21.733	1.00	19.8
165	ND2	ASN	A	834	10.764	0.183	20.928	1.00	19.76
166	N	PHE	A	835	15.868	-1.11	20.954	1.00	22.4
167	CA	PHE	A	835	17.15	-0.401	20.982	1.00	22.69
168	C	PHE	A	835	18.104	-1.186	20.091	1.00	23.14
169	O	PHE	A	835	19.148	-0.682	19.669	1.00	23.31
170	CB	PHE	A	835	17.734	-0.325	22.402	1.00	21.96
171	CG	PHE	A	835	17.17	0.797	23.23	1.00	21.74
172	CD1	PHE	A	835	16.122	0.572	24.117	1.00	21.46
173	CD2	PHE	A	835	17.673	2.089	23.102	1.00	21.17
174	CE1	PHE	A	835	15.586	1.617	24.862	1.00	21.31
175	CE2	PHE	A	835	17.144	3.136	23.839	1.00	21.13
176	CZ	PHE	A	835	16.099	2.901	24.721	1.00	21.32
177	N	GLY	A	836	17.726	-2.429	19.809	1.00	23.62
178	CA	GLY	A	836	18.544	-3.287	18.977	1.00	24.16
179	C	GLY	A	836	19.685	-3.867	19.785	1.00	24.74
180	O	GLY	A	836	19.506	-4.23	20.951	1.00	24.71
181	N	GLN	A	837	20.856	-3.958	19.165	1.00	25.05
182	CA	GLN	A	837	22.041	-4.486	19.825	1.00	25.41
183	C	GLN	A	837	22.737	-3.373	20.606	1.00	25.32
184	O	GLN	A	837	23.061	-2.319	20.055	1.00	25.12
185	CB	GLN	A	837	23.008	-5.071	18.786	1.00	26.25
186	CG	GLN	A	837	22.465	-6.276	18.033	1.00	26.72
187	CD	GLN	A	837	22.203	-7.455	18.945	1.00	27.42
188	OE1	GLN	A	837	23.118	-7.97	19.587	1.00	28.28
189	NE2	GLN	A	837	20.948	-7.892	19.011	1.00	27.69
190	N	VAL	A	838	22.953	-3.612	21.894	1.00	25.13
191	CA	VAL	A	838	23.614	-2.644	22.759	1.00	24.79
192	C	VAL	A	838	24.686	-3.353	23.575	1.00	24.66
193	O	VAL	A	838	24.713	-4.581	23.649	1.00	24.5
194	CB	VAL	A	838	22.613	-1.974	23.722	1.00	24.81
195	CG1	VAL	A	838	21.584	-1.187	22.929	1.00	25.33
196	CG2	VAL	A	838	21.922	-3.028	24.579	1.00	25.05
197	N	LEU	A	839	25.568	-2.574	24.187	1.00	24.68
198	CA	LEU	A	839	26.646	-3.132	24.991	1.00	24.69
199	C	LEU	A	839	26.348	-3.045	26.48	1.00	24.54

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

200	O	LEU	A	839	26.024	-1.974	26.991	1.00	24.64
201	CB	LEU	A	839	27.945	-2.377	24.707	1.00	24.91
202	CG	LEU	A	839	28.564	-2.549	23.321	1.00	25.23
203	CD1	LEU	A	839	29.481	-1.373	23.022	1.00	25.5
204	CD2	LEU	A	839	29.323	-3.865	23.257	1.00	25.27
205	N	LYS	A	840	26.441	-4.166	27.183	1.00	24.51
206	CA	LYS	A	840	26.225	-4.122	28.619	1.00	24.73
207	C	LYS	A	840	27.464	-3.42	29.156	1.00	24.58
208	O	LYS	A	840	28.564	-3.632	28.645	1.00	24.3
209	CB	LYS	A	840	26.149	-5.52	29.231	1.00	25.33
210	CG	LYS	A	840	25.909	-5.469	30.734	1.00	26.1
211	CD	LYS	A	840	26.196	-6.792	31.423	1.00	27.67
212	CE	LYS	A	840	25.942	-6.672	32.927	1.00	28.08
213	NZ	LYS	A	840	26.563	-7.783	33.703	1.00	29.12
214	N	ALA	A	841	27.301	-2.593	30.181	1.00	24.39
215	CA	ALA	A	841	28.445	-1.884	30.731	1.00	24.53
216	C	ALA	A	841	28.231	-1.363	32.143	1.00	24.67
217	O	ALA	A	841	27.175	-1.544	32.751	1.00	24.28
218	CB	ALA	A	841	28.819	-0.722	29.814	1.00	24.28
219	N	ARG	A	842	29.268	-0.719	32.658	1.00	25.04
220	CA	ARG	A	842	29.226	-0.122	33.973	1.00	25.71
221	C	ARG	A	842	29.631	1.324	33.751	1.00	25.87
222	O	ARG	A	842	30.584	1.602	33.022	1.00	25.77
223	CB	ARG	A	842	30.213	-0.808	34.917	1.00	26.17
224	CG	ARG	A	842	30.054	-2.318	35.007	1.00	26.74
225	CD	ARG	A	842	29.972	-2.764	36.453	1.00	27.24
226	NE	ARG	A	842	28.638	-2.562	37.013	1.00	27.81
227	CZ	ARG	A	842	28.387	-1.975	38.181	1.00	27.67
228	NH1	ARG	A	842	29.38	-1.514	38.927	1.00	27.41
229	NH2	ARG	A	842	27.137	-1.871	38.611	1.00	27.79
230	N	ILE	A	843	28.897	2.241	34.361	1.00	26.06
231	CA	ILE	A	843	29.19	3.653	34.215	1.00	26.89
232	C	ILE	A	843	29.262	4.312	35.579	1.00	27.74
233	O	ILE	A	843	29.061	3.678	36.612	1.00	27.29
234	CB	ILE	A	843	28.095	4.375	33.406	1.00	26.63
235	CG1	ILE	A	843	26.766	4.3	34.16	1.00	26.53
236	CG2	ILE	A	843	27.964	3.742	32.024	1.00	26.95
237	CD1	ILE	A	843	25.651	5.131	33.549	1.00	26.59
238	N	LYS	A	844	29.547	5.602	35.57	1.00	29.04
239	CA	LYS	A	844	29.619	6.354	36.802	1.00	30.6

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## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

240	C	LYS	A	844	28.628	7.49	36.65	1.00	31.15
241	O	LYS	A	844	28.742	8.309	35.735	1.00	31.49
242	CB	LYS	A	844	31.031	6.895	37.009	1.00	31.38
243	CG	LYS	A	844	31.334	7.351	38.429	1.00	33.01
244	CD	LYS	A	844	32.834	7.594	38.605	1.00	33.67
245	CE	LYS	A	844	33.174	8.079	40.005	1.00	34.28
246	NZ	LYS	A	844	34.646	8.295	40.176	1.00	34.73
247	N	LYS	A	845	27.63	7.511	37.523	1.00	31.58
248	CA	LYS	A	845	26.632	8.559	37.483	1.00	32.19
249	C	LYS	A	845	26.446	9.105	38.888	1.00	32.67
250	O	LYS	A	845	26.303	8.345	39.848	1.00	32.57
251	CB	LYS	A	845	25.298	8.029	36.95	1.00	32.49
252	CG	LYS	A	845	24.369	9.152	36.515	1.00	32.67
253	CD	LYS	A	845	22.959	8.686	36.218	1.00	33.12
254	CE	LYS	A	845	22.104	9.868	35.774	1.00	33.05
255	NZ	LYS	A	845	20.678	9.509	35.651	1.00	33.81
256	N	ASP	A	846	26.454	10.429	38.998	1.00	33.23
257	CA	ASP	A	846	26.298	11.105	40.28	1.00	33.68
258	C	ASP	A	846	27.342	10.594	41.264	1.00	33.59
259	O	ASP	A	846	27.07	10.447	42.459	1.00	33.51
260	CB	ASP	A	846	24.892	10.874	40.843	1.00	34.37
261	CG	ASP	A	846	23.803	11.274	39.866	1.00	35.04
262	OD1	ASP	A	846	23.997	12.267	39.13	1.00	35.41
263	OD2	ASP	A	846	22.752	10.6	39.841	1.00	35.47
264	N	GLY	A	847	28.532	10.309	40.74	1.00	33.24
265	CA	GLY	A	847	29.619	9.832	41.573	1.00	32.82
266	C	GLY	A	847	29.605	8.354	41.901	1.00	32.53
267	O	GLY	A	847	30.596	7.835	42.403	1.00	32.65
268	N	LEU	A	848	28.503	7.664	41.624	1.00	32.36
269	CA	LEU	A	848	28.44	6.241	41.933	1.00	32.14
270	C	LEU	A	848	28.456	5.317	40.715	1.00	31.95
271	O	LEU	A	848	28.17	5.73	39.591	1.00	31.73
272	CB	LEU	A	848	27.222	5.943	42.817	1.00	32.5
273	CG	LEU	A	848	27.301	6.577	44.217	1.00	32.88
274	CD1	LEU	A	848	26.079	6.188	45.039	1.00	33.02
275	CD2	LEU	A	848	28.581	6.125	44.925	1.00	32.91
276	N	ARG	A	849	28.796	4.057	40.973	1.00	31.47
277	CA	ARG	A	849	28.909	3.022	39.952	1.00	30.98
278	C	ARG	A	849	27.596	2.263	39.777	1.00	30.13
279	O	ARG	A	849	26.924	1.958	40.759	1.00	29.94

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TABLE 4  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

280	CB	ARG	A	849	30.009	2.04	40.364	1.00	31.97
281	CG	ARG	A	849	30.708	1.372	39.212	1.00	33.46
282	CD	ARG	A	849	31.63	2.36	38.519	1.00	34.61
283	NE	ARG	A	849	32.042	1.881	37.204	1.00	35.35
284	CZ	ARG	A	849	32.793	2.576	36.36	1.00	35.49
285	NH1	ARG	A	849	33.113	2.063	35.184	1.00	35.85
286	NH2	ARG	A	849	33.228	3.783	36.698	1.00	35.57
287	N	MET	A	850	27.244	1.94	38.533	1.00	28.96
288	CA	MET	A	850	26.002	1.218	38.264	1.00	27.64
289	C	MET	A	850	26.004	0.507	36.912	1.00	26.97
290	O	MET	A	850	26.821	0.808	36.034	1.00	26.45
291	CB	MET	A	850	24.818	2.189	38.31	1.00	27.34
292	CG	MET	A	850	24.806	3.195	37.16	1.00	26.87
293	SD	MET	A	850	23.435	4.358	37.258	1.00	26.63
294	CE	MET	A	850	22.006	3.251	36.967	1.00	26.01
295	N	ASP	A	851	25.084	-0.441	36.756	1.00	26.18
296	CA	ASP	A	851	24.955	-1.169	35.502	1.00	25.56
297	C	ASP	A	851	24.267	-0.258	34.499	1.00	25.06
298	O	ASP	A	851	23.583	0.692	34.877	1.00	24.92
299	CB	ASP	A	851	24.101	-2.43	35.665	1.00	25.71
300	CG	ASP	A	851	24.805	-3.514	36.461	1.00	26.28
301	OD1	ASP	A	851	26.052	-3.528	36.485	1.00	26.4
302	OD2	ASP	A	851	24.105	-4.366	37.052	1.00	26.51
303	N	ALA	A	852	24.454	-0.554	33.22	1.00	24.42
304	CA	ALA	A	852	23.833	0.219	32.16	1.00	24.04
305	C	ALA	A	852	24.055	-0.484	30.834	1.00	23.71
306	O	ALA	A	852	24.918	-1.353	30.717	1.00	23.49
307	CB	ALA	A	852	24.429	1.626	32.108	1.00	23.84
308	N	ALA	A	853	23.253	-0.121	29.845	1.00	23.36
309	CA	ALA	A	853	23.398	-0.673	28.505	1.00	23.62
310	C	ALA	A	853	23.824	0.528	27.671	1.00	23.59
311	O	ALA	A	853	23.431	1.657	27.962	1.00	23.22
312	CB	ALA	A	853	22.074	-1.238	28.001	1.00	23.3
313	N	ILE	A	854	24.635	0.298	26.646	1.00	23.89
314	CA	ILE	A	854	25.098	1.4	25.825	1.00	24.38
315	C	ILE	A	854	24.921	1.18	24.327	1.00	25.1
316	O	ILE	A	854	25.393	0.2	23.749	1.00	24.64
317	CB	ILE	A	854	26.577	1.727	26.145	1.00	24.24
318	CG1	ILE	A	854	26.673	2.273	27.573	1.00	24.11
319	CG2	ILE	A	854	27.134	2.739	25.142	1.00	24.15

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TABLE 4  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

320	CD1	ILE	A	854	28.083	2.482	28.062	1.00	24.02
321	N	LYS	A	855	24.217	2.123	23.72	1.00	26
322	CA	LYS	A	855	23.937	2.115	22.298	1.00	27.38
323	C	LYS	A	855	24.921	3.087	21.637	1.00	28.14
324	O	LYS	A	855	24.937	4.275	21.97	1.00	27.78
325	CB	LYS	A	855	22.492	2.585	22.08	1.00	27.39
326	CG	LYS	A	855	22.058	2.774	20.632	1.00	27.75
327	CD	LYS	A	855	21.637	1.463	20.002	1.00	28.56
328	CE	LYS	A	855	20.897	1.692	18.692	1.00	28.57
329	NZ	LYS	A	855	20.671	0.404	17.984	1.00	29.06
330	N	ARG	A	856	25.75	2.584	20.725	1.00	29.36
331	CA	ARG	A	856	26.706	3.44	20.026	1.00	30.95
332	C	ARG	A	856	26.098	3.891	18.705	1.00	31.92
333	O	ARG	A	856	25.619	3.076	17.923	1.00	31.87
334	CB	ARG	A	856	28.024	2.707	19.753	1.00	30.95
335	CG	ARG	A	856	29.088	3.599	19.104	1.00	31.73
336	CD	ARG	A	856	30.403	2.86	18.886	1.00	32.59
337	NE	ARG	A	856	30.264	1.803	17.892	1.00	33.62
338	CZ	ARG	A	856	31.067	0.747	17.798	1.00	34.27
339	NH1	ARG	A	856	32.078	0.595	18.643	1.00	34.4
340	NH2	ARG	A	856	30.857	-0.16	16.852	1.00	35.04
341	N	MET	A	857	26.134	5.194	18.459	1.00	33.46
342	CA	MET	A	857	25.564	5.761	17.243	1.00	34.97
343	C	MET	A	857	26.558	6.713	16.582	1.00	35.74
344	O	MET	A	857	27.172	7.544	17.254	1.00	35.47
345	CB	MET	A	857	24.273	6.505	17.596	1.00	35.41
346	CG	MET	A	857	23.269	5.654	18.372	1.00	36.27
347	SD	MET	A	857	21.942	6.603	19.169	1.00	37.78
348	CE	MET	A	857	20.798	6.799	17.816	1.00	37.34
349	N	ALA	A	858	26.717	6.586	15.267	1.00	36.84
350	CA	ALA	A	858	27.637	7.443	14.525	1.00	38.43
351	C	ALA	A	858	27.055	8.851	14.436	1.00	39.57
352	O	ALA	A	858	25.837	9.025	14.378	1.00	39.67
353	CB	ALA	A	858	27.878	6.876	13.127	1.00	38.26
354	N	GLU	A	859	27.929	9.854	14.437	1.00	41.14
355	CA	GLU	A	859	27.495	11.25	14.369	1.00	42.68
356	C	GLU	A	859	27.723	11.871	12.992	1.00	43.39
357	O	GLU	A	859	28.498	12.818	12.84	1.00	43.68
358	CB	GLU	A	859	28.217	12.075	15.44	1.00	43.12
359	CG	GLU	A	859	27.853	11.675	16.864	1.00	43.91



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TABLE 4  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

360	CD	GLU	A	859	28.588	12.485	17.909	1.00	44.22
361	OE1	GLU	A	859	29.83	12.372	17.98	1.00	44.86
362	OE2	GLU	A	859	27.926	13.234	18.661	1.00	44.7
363	N	ALA	A	860	27.025	11.331	11.997	1.00	44.07
364	CA	ALA	A	860	27.117	11.795	10.617	1.00	44.63
365	CB	ALA	A	860	28.577	11.875	10.175	1.00	44.72
366	C	ALA	A	860	26.362	10.805	9.739	1.00	45.04
367	OT1	ALA	A	860	27.036	10.085	8.969	1.00	45.39
368	OT2	ALA	A	860	25.116	10.746	9.849	1.00	45.21
369	N	ALA	A	867	19.562	15.55	10.383	1.00	68.36
370	CA	ALA	A	867	19.174	14.375	9.549	1.00	68.35
371	C	ALA	A	867	18.375	13.358	10.365	1.00	68.25
372	O	ALA	A	867	17.584	13.73	11.234	1.00	68.27
373	CB	ALA	A	867	20.425	13.716	8.966	1.00	68.41
374	N	ASP	A	868	18.584	12.076	10.073	1.00	68.09
375	CA	ASP	A	868	17.891	10.991	10.77	1.00	67.86
376	C	ASP	A	868	18.343	10.92	12.228	1.00	67.51
377	O	ASP	A	868	17.543	10.659	13.13	1.00	67.5
378	CB	ASP	A	868	18.183	9.656	10.071	1.00	68.05
379	CG	ASP	A	868	17.421	8.491	10.683	1.00	68.2
380	OD1	ASP	A	868	17.611	8.209	11.887	1.00	68.26
381	OD2	ASP	A	868	16.632	7.854	9.952	1.00	68.31
382	N	PHE	A	869	19.634	11.15	12.441	1.00	67.04
383	CA	PHE	A	869	20.234	11.126	13.771	1.00	66.56
384	C	PHE	A	869	19.49	12.066	14.72	1.00	66.06
385	O	PHE	A	869	18.918	11.633	15.725	1.00	65.94
386	CB	PHE	A	869	21.705	11.544	13.67	1.00	66.86
387	CG	PHE	A	869	22.423	11.583	14.989	1.00	67.01
388	CD1	PHE	A	869	22.616	10.421	15.727	1.00	67.05
389	CD2	PHE	A	869	22.922	12.785	15.484	1.00	67.14
390	CE1	PHE	A	869	23.298	10.453	16.941	1.00	67.16
391	CE2	PHE	A	869	23.607	12.829	16.699	1.00	67.21
392	CZ	PHE	A	869	23.796	11.66	17.428	1.00	67.24
393	N	ALA	A	870	19.504	13.354	14.388	1.00	65.35
394	CA	ALA	A	870	18.845	14.376	15.194	1.00	64.65
395	C	ALA	A	870	17.38	14.039	15.468	1.00	64.05
396	O	ALA	A	870	16.848	14.37	16.527	1.00	64
397	CB	ALA	A	870	18.948	15.73	14.497	1.00	64.66
398	N	GLY	A	871	16.734	13.38	14.511	1.00	63.31
399	CA	GLY	A	871	15.337	13.02	14.675	1.00	62.29

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TABLE 4  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

400	C	GLY	A	871	15.062	12.167	15.899	1.00	61.61
401	O	GLY	A	871	14.363	12.597	16.819	1.00	61.54
402	N	GLU	A	872	15.616	10.958	15.913	1.00	60.78
403	CA	GLU	A	872	15.424	10.028	17.022	1.00	59.95
404	C	GLU	A	872	15.889	10.589	18.363	1.00	59.15
405	O	GLU	A	872	15.198	10.452	19.373	1.00	59
406	CB	GLU	A	872	16.154	8.717	16.729	1.00	60.16
407	CG	GLU	A	872	15.71	8.062	15.436	1.00	60.61
408	CD	GLU	A	872	16.432	6.761	15.16	1.00	60.98
409	OE1	GLU	A	872	17.681	6.778	15.073	1.00	61.1
410	OE2	GLU	A	872	15.749	5.722	15.028	1.00	61.14
411	N	LEU	A	873	17.062	11.213	18.37	1.00	58.23
412	CA	LEU	A	873	17.613	11.795	19.589	1.00	57.28
413	C	LEU	A	873	16.673	12.89	20.097	1.00	56.53
414	O	LEU	A	873	16.518	13.091	21.303	1.00	56.5
415	CB	LEU	A	873	18.997	12.382	19.302	1.00	57.45
416	CG	LEU	A	873	19.816	12.883	20.493	1.00	57.62
417	CD1	LEU	A	873	20.157	11.715	21.412	1.00	57.49
418	CD2	LEU	A	873	21.089	13.553	19.987	1.00	57.7
419	N	GLU	A	874	16.046	13.587	19.155	1.00	55.58
420	CA	GLU	A	874	15.107	14.663	19.453	1.00	54.47
421	C	GLU	A	874	13.886	14.126	20.204	1.00	53.38
422	O	GLU	A	874	13.257	14.843	20.986	1.00	53.15
423	CB	GLU	A	874	14.679	15.327	18.138	1.00	55.06
424	CG	GLU	A	874	13.637	16.423	18.253	1.00	55.7
425	CD	GLU	A	874	13.345	17.073	16.908	1.00	56.22
426	OE1	GLU	A	874	14.248	17.744	16.363	1.00	56.4
427	OE2	GLU	A	874	12.217	16.907	16.391	1.00	56.47
428	N	VAL	A	875	13.561	12.86	19.965	1.00	51.97
429	CA	VAL	A	875	12.424	12.223	20.617	1.00	50.57
430	C	VAL	A	875	12.828	11.591	21.948	1.00	49.41
431	O	VAL	A	875	12.05	11.582	22.901	1.00	49.12
432	CB	VAL	A	875	11.807	11.135	19.712	1.00	50.7
433	CG1	VAL	A	875	10.648	10.457	20.424	1.00	50.6
434	CG2	VAL	A	875	11.336	11.757	18.406	1.00	50.69
435	N	LEU	A	876	14.048	11.068	22.011	1.00	48.11
436	CA	LEU	A	876	14.536	10.441	23.23	1.00	46.91
437	C	LEU	A	876	14.56	11.417	24.397	1.00	45.98
438	O	LEU	A	876	14.249	11.043	25.528	1.00	45.99
439	CB	LEU	A	876	15.935	9.861	23.011	1.00	46.81

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TABLE 4  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

440	CG	LEU	A	876	16.017	8.688	22.03	1.00	46.65
441	CD1	LEU	A	876	17.461	8.215	21.909	1.00	46.79
442	CD2	LEU	A	876	15.119	7.554	22.512	1.00	46.84
443	N	CYS	A	877	14.921	12.668	24.123	1.00	44.82
444	CA	CYS	A	877	14.981	13.689	25.167	1.00	43.66
445	C	CYS	A	877	13.606	14.011	25.746	1.00	42.37
446	O	CYS	A	877	13.493	14.392	26.908	1.00	42.29
447	CB	CYS	A	877	15.616	14.968	24.62	1.00	44.16
448	SG	CYS	A	877	17.314	14.749	24.047	1.00	45.25
449	N	LYS	A	878	12.568	13.854	24.93	1.00	40.94
450	CA	LYS	A	878	11.193	14.124	25.351	1.00	39.51
451	C	LYS	A	878	10.618	13.044	26.27	1.00	38.16
452	O	LYS	A	878	9.574	13.242	26.899	1.00	38.04
453	CB	LYS	A	878	10.292	14.262	24.12	1.00	40.1
454	CG	LYS	A	878	10.458	15.561	23.35	1.00	40.56
455	CD	LYS	A	878	9.959	16.735	24.179	1.00	41.37
456	CE	LYS	A	878	10.038	18.044	23.413	1.00	41.69
457	NZ	LYS	A	878	9.454	19.16	24.211	1.00	42.1
458	N	LEU	A	879	11.298	11.903	26.344	1.00	36.44
459	CA	LEU	A	879	10.838	10.788	27.164	1.00	34.64
460	C	LEU	A	879	10.642	11.107	28.637	1.00	33.28
461	O	LEU	A	879	9.702	10.611	29.259	1.00	33
462	CB	LEU	A	879	11.804	9.603	27.042	1.00	34.96
463	CG	LEU	A	879	11.773	8.817	25.73	1.00	34.99
464	CD1	LEU	A	879	12.844	7.736	25.754	1.00	35.17
465	CD2	LEU	A	879	10.395	8.205	25.54	1.00	34.76
466	N	GLY	A	880	11.52	11.935	29.194	1.00	31.44
467	CA	GLY	A	880	11.416	12.25	30.604	1.00	29.58
468	C	GLY	A	880	11.842	11.023	31.395	1.00	28.38
469	O	GLY	A	880	12.605	10.195	30.896	1.00	28.21
470	N	HIS	A	881	11.349	10.89	32.621	1.00	26.99
471	CA	HIS	A	881	11.704	9.747	33.452	1.00	25.72
472	C	HIS	A	881	10.471	9.114	34.088	1.00	24.34
473	O	HIS	A	881	9.574	9.81	34.577	1.00	23.89
474	CB	HIS	A	881	12.695	10.169	34.54	1.00	26.29
475	CG	HIS	A	881	13.983	10.71	34.001	1.00	27.29
476	ND1	HIS	A	881	14.878	9.937	33.29	1.00	27.59
477	CD2	HIS	A	881	14.516	11.956	34.047	1.00	27.49
478	CE1	HIS	A	881	15.907	10.682	32.924	1.00	27.67
479	NE2	HIS	A	881	15.711	11.912	33.371	1.00	27.64

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TABLE 4

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

480	N	HIS	A	882	10.439	7.785	34.07	1.00	22.36
481	CA	HIS	A	882	9.328	7.036	34.637	1.00	20.38
482	C	HIS	A	882	9.774	5.612	34.966	1.00	19.21
483	O	HIS	A	882	10.583	5.021	34.252	1.00	18.66
484	CB	HIS	A	882	8.154	7.017	33.653	1.00	19.74
485	CG	HIS	A	882	6.909	6.415	34.221	1.00	19.47
486	ND1	HIS	A	882	6.729	5.054	34.341	1.00	19.14
487	CD2	HIS	A	882	5.807	6.99	34.756	1.00	19.18
488	CE1	HIS	A	882	5.569	4.817	34.926	1.00	19.29
489	NE2	HIS	A	882	4.99	5.975	35.188	1.00	19.38
490	N	PRO	A	883	9.247	5.043	36.061	1.00	18.27
491	CA	PRO	A	883	9.586	3.684	36.502	1.00	17.59
492	C	PRO	A	883	9.379	2.575	35.464	1.00	16.82
493	O	PRO	A	883	10.139	1.609	35.423	1.00	16.33
494	CB	PRO	A	883	8.676	3.474	37.715	1.00	17.72
495	CG	PRO	A	883	8.462	4.855	38.235	1.00	18.04
496	CD	PRO	A	883	8.28	5.667	36.983	1.00	18.06
497	N	ASN	A	884	8.364	2.716	34.619	1.00	15.97
498	CA	ASN	A	884	8.072	1.665	33.657	1.00	15.58
499	C	ASN	A	884	8.498	1.856	32.202	1.00	15.55
500	O	ASN	A	884	7.964	1.219	31.293	1.00	15.53
501	CB	ASN	A	884	6.588	1.322	33.765	1.00	14.98
502	CG	ASN	A	884	6.196	0.948	35.191	1.00	15.09
503	OD1	ASN	A	884	5.389	1.63	35.834	1.00	14.89
504	ND2	ASN	A	884	6.785	-0.132	35.7	1.00	14.54
505	N	ILE	A	885	9.479	2.724	31.986	1.00	15.73
506	CA	ILE	A	885	10.012	2.948	30.648	1.00	15.69
507	C	ILE	A	885	11.526	2.773	30.788	1.00	15.88
508	O	ILE	A	885	12.048	2.841	31.902	1.00	15.47
509	CB	ILE	A	885	9.726	4.381	30.146	1.00	15.81
510	CG1	ILE	A	885	10.519	5.398	30.972	1.00	16.14
511	CG2	ILE	A	885	8.234	4.682	30.233	1.00	15.67
512	CD1	ILE	A	885	10.456	6.812	30.42	1.00	16.56
513	N	ILE	A	886	12.23	2.514	29.69	1.00	15.97
514	CA	ILE	A	886	13.682	2.408	29.778	1.00	15.97
515	C	ILE	A	886	14.145	3.853	29.871	1.00	16.72
516	O	ILE	A	886	13.894	4.655	28.974	1.00	16.5
517	CB	ILE	A	886	14.317	1.764	28.532	1.00	15.7
518	CG1	ILE	A	886	14.046	0.257	28.525	1.00	15.45
519	CG2	ILE	A	886	15.826	2.037	28.518	1.00	15.41

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TABLE 4

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

520	CD1	ILE	A	886	14.594	-0.466	29.744	1.00	15.66
521	N	ASN	A	887	14.803	4.184	30.973	1.00	17.46
522	CA	ASN	A	887	15.267	5.539	31.194	1.00	18.24
523	C	ASN	A	887	16.681	5.799	30.686	1.00	18.68
524	O	ASN	A	887	17.537	4.915	30.684	1.00	18
525	CB	ASN	A	887	15.191	5.861	32.688	1.00	18.97
526	CG	ASN	A	887	13.758	5.909	33.205	1.00	19.42
527	OD1	ASN	A	887	13.025	6.864	32.946	1.00	20.22
528	ND2	ASN	A	887	13.353	4.873	33.93	1.00	19.44
529	N	LEU	A	888	16.901	7.031	30.245	1.00	19.25
530	CA	LEU	A	888	18.201	7.465	29.769	1.00	20.11
531	C	LEU	A	888	19.019	7.806	31.013	1.00	20.3
532	O	LEU	A	888	18.551	8.537	31.88	1.00	20.31
533	CB	LEU	A	888	18.058	8.715	28.903	1.00	20.77
534	CG	LEU	A	888	19.384	9.429	28.641	1.00	21.82
535	CD1	LEU	A	888	20.305	8.487	27.909	1.00	22.55
536	CD2	LEU	A	888	19.165	10.701	27.836	1.00	22.92
537	N	LEU	A	889	20.232	7.278	31.1	1.00	20.51
538	CA	LEU	A	889	21.079	7.541	32.247	1.00	21.14
539	C	LEU	A	889	22.057	8.676	31.943	1.00	21.91
540	O	LEU	A	889	22.475	9.4	32.843	1.00	22.33
541	CB	LEU	A	889	21.832	6.262	32.637	1.00	20.89
542	CG	LEU	A	889	20.909	5.08	32.97	1.00	21.15
543	CD1	LEU	A	889	21.717	3.813	33.23	1.00	20.91
544	CD2	LEU	A	889	20.066	5.438	34.193	1.00	21.07
545	N	GLY	A	890	22.408	8.836	30.67	1.00	22.24
546	CA	GLY	A	890	23.335	9.887	30.288	1.00	22.72
547	C	GLY	A	890	23.924	9.604	28.923	1.00	22.88
548	O	GLY	A	890	23.593	8.598	28.304	1.00	23
549	N	ALA	A	891	24.794	10.484	28.444	1.00	23.48
550	CA	ALA	A	891	25.407	10.292	27.133	1.00	23.8
551	C	ALA	A	891	26.839	10.803	27.069	1.00	24.3
552	O	ALA	A	891	27.219	11.724	27.795	1.00	23.94
553	CB	ALA	A	891	24.572	10.966	26.067	1.00	23.59
554	N	CYS	A	892	27.621	10.195	26.183	1.00	24.83
555	CA	CYS	A	892	29.019	10.558	25.992	1.00	25.76
556	C	CYS	A	892	29.386	10.636	24.51	1.00	26.43
557	O	CYS	A	892	29.183	9.68	23.76	1.00	26.36
558	CB	CYS	A	892	29.926	9.527	26.682	1.00	25.52
559	SG	CYS	A	892	31.699	9.676	26.307	1.00	25.7

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TABLE 4

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

560	N	GLU	A	893	29.908	11.782	24.086	1.00	27.33
561	CA	GLU	A	893	30.336	11.946	22.702	1.00	28.61
562	C	GLU	A	893	31.83	11.646	22.706	1.00	28.67
563	O	GLU	A	893	32.585	12.255	23.465	1.00	28.38
564	CB	GLU	A	893	30.098	13.377	22.218	1.00	29.72
565	CG	GLU	A	893	28.648	13.808	22.273	1.00	32.07
566	CD	GLU	A	893	28.439	15.215	21.749	1.00	33.39
567	OE1	GLU	A	893	29.094	16.151	22.26	1.00	34.27
568	OE2	GLU	A	893	27.611	15.384	20.826	1.00	34.39
569	N	HIS	A	894	32.254	10.707	21.866	1.00	28.96
570	CA	HIS	A	894	33.657	10.323	21.818	1.00	29.51
571	C	HIS	A	894	34.152	10.001	20.405	1.00	30.53
572	O	HIS	A	894	33.643	9.096	19.734	1.00	30.17
573	CB	HIS	A	894	33.881	9.108	22.731	1.00	28.56
574	CG	HIS	A	894	35.324	8.794	22.988	1.00	27.76
575	ND1	HIS	A	894	36.133	9.589	23.77	1.00	27.32
576	CD2	HIS	A	894	36.094	7.757	22.583	1.00	27.1
577	CE1	HIS	A	894	37.339	9.056	23.839	1.00	26.59
578	NE2	HIS	A	894	37.342	7.945	23.127	1.00	26.84
579	N	ARG	A	895	35.149	10.761	19.97	1.00	31.87
580	CA	ARG	A	895	35.77	10.582	18.666	1.00	33.44
581	C	ARG	A	895	34.837	10.187	17.526	1.00	34.6
582	O	ARG	A	895	35.048	9.17	16.868	1.00	34.55
583	CB	ARG	A	895	36.898	9.559	18.793	1.00	33.43
584	CG	ARG	A	895	37.972	9.974	19.782	1.00	33.79
585	CD	ARG	A	895	38.718	11.209	19.288	1.00	34.22
586	NE	ARG	A	895	39.828	11.58	20.163	1.00	34.56
587	CZ	ARG	A	895	40.729	12.515	19.869	1.00	35
588	NH1	ARG	A	895	41.709	12.794	20.723	1.00	34.72
589	NH2	ARG	A	895	40.656	13.17	18.716	1.00	34.77
590	N	GLY	A	896	33.804	10.992	17.303	1.00	36.14
591	CA	GLY	A	896	32.88	10.729	16.216	1.00	38.33
592	C	GLY	A	896	31.655	9.884	16.492	1.00	40.07
593	O	GLY	A	896	30.815	9.718	15.609	1.00	40.16
594	N	PTY	A	897	31.53	9.35	17.701	1.00	41.79
595	CA	PTY	A	897	30.378	8.519	18.017	1.00	43.46
596	CB	PTY	A	897	30.813	7.05	18.126	1.00	49.9
597	CG	PTY	A	897	31.41	6.485	16.848	1.00	57.56
598	CD1	PTY	A	897	30.613	5.848	15.899	1.00	61.09
599	CE1	PTY	A	897	31.158	5.352	14.712	1.00	66.64

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TABLE 4

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

600	CD2	PTY	A	897	32.769	6.612	16.578	1.00	61.22
601	CE2	PTY	A	897	33.325	6.125	15.399	1.00	66.71
602	CZ	PTY	A	897	32.521	5.492	14.459	1.00	69.6
603	OH	PTY	A	897	33.147	4.985	13.105	1.00	80.34
604	PR	PTY	A	897	34.693	5.22	12.559	0.25	77.87
605	OR1	PTY	A	897	34.655	4.599	11.212	0.25	78.81
606	OR2	PTY	A	897	35.544	4.505	13.543	0.25	78.77
607	OR3	PTY	A	897	34.845	6.696	12.552	0.25	78.77
608	C	PTY	A	897	29.679	8.957	19.3	1.00	40.91
609	O	PTY	A	897	30.31	9.466	20.226	1.00	40.55
610	N	LEU	A	898	28.363	8.779	19.332	1.00	37.9
611	CA	LEU	A	898	27.575	9.12	20.506	1.00	34.93
612	C	LEU	A	898	27.278	7.821	21.234	1.00	32.84
613	O	LEU	A	898	26.744	6.874	20.649	1.00	32.62
614	CB	LEU	A	898	26.253	9.787	20.121	1.00	34.9
615	CG	LEU	A	898	25.346	10.101	21.319	1.00	34.71
616	CD1	LEU	A	898	25.89	11.302	22.077	1.00	34.57
617	CD2	LEU	A	898	23.936	10.381	20.841	1.00	34.99
618	N	TYR	A	899	27.63	7.782	22.511	1.00	30.09
619	CA	TYR	A	899	27.41	6.606	23.332	1.00	27.53
620	C	TYR	A	899	26.293	6.913	24.32	1.00	26.34
621	O	TYR	A	899	26.489	7.632	25.301	1.00	25.86
622	CB	TYR	A	899	28.704	6.241	24.055	1.00	26.62
623	CG	TYR	A	899	29.804	5.817	23.104	1.00	25.74
624	CD1	TYR	A	899	30.064	4.468	22.864	1.00	25.2
625	CD2	TYR	A	899	30.565	6.768	22.418	1.00	25.09
626	CE1	TYR	A	899	31.055	4.072	21.968	1.00	24.73
627	CE2	TYR	A	899	31.556	6.387	21.519	1.00	24.77
628	CZ	TYR	A	899	31.796	5.036	21.302	1.00	24.89
629	OH	TYR	A	899	32.784	4.657	20.433	1.00	24.59
630	N	LEU	A	900	25.12	6.362	24.036	1.00	24.87
631	CA	LEU	A	900	23.936	6.571	24.851	1.00	23.68
632	C	LEU	A	900	23.793	5.503	25.93	1.00	22.88
633	O	LEU	A	900	23.674	4.315	25.629	1.00	22.41
634	CB	LEU	A	900	22.703	6.558	23.955	1.00	23.88
635	CG	LEU	A	900	21.371	6.896	24.615	1.00	24.34
636	CD1	LEU	A	900	21.361	8.364	25.028	1.00	24.04
637	CD2	LEU	A	900	20.251	6.613	23.634	1.00	24.4
638	N	ALA	A	901	23.811	5.933	27.188	1.00	21.78
639	CA	ALA	A	901	23.676	5.012	28.308	1.00	20.98

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## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

640	C	ALA	A	901	22.218	4.945	28.748	1.00	20.35
641	O	ALA	A	901	21.62	5.964	29.093	1.00	20.33
642	CB	ALA	A	901	24.55	5.464	29.47	1.00	20.6
643	N	ILE	A	902	21.65	3.746	28.719	1.00	19.58
644	CA	ILE	A	902	20.267	3.544	29.124	1.00	19.34
645	C	ILE	A	902	20.23	2.484	30.21	1.00	19.07
646	O	ILE	A	902	21.234	1.823	30.476	1.00	18.81
647	CB	ILE	A	902	19.373	3.076	27.946	1.00	19.43
648	CG1	ILE	A	902	19.893	1.752	27.386	1.00	19.23
649	CG2	ILE	A	902	19.331	4.149	26.869	1.00	19.23
650	CD1	ILE	A	902	19.039	1.17	26.274	1.00	19.43
651	N	GLU	A	903	19.07	2.321	30.831	1.00	18.74
652	CA	GLU	A	903	18.928	1.349	31.902	1.00	19.01
653	C	GLU	A	903	19.146	-0.083	31.46	1.00	18.7
654	O	GLU	A	903	18.792	-0.468	30.349	1.00	18.55
655	CB	GLU	A	903	17.557	1.481	32.562	1.00	19.1
656	CG	GLU	A	903	17.479	2.616	33.563	1.00	19.78
657	CD	GLU	A	903	16.104	2.75	34.177	1.00	20.34
658	OE1	GLU	A	903	16.006	3.305	35.292	1.00	21.39
659	OE2	GLU	A	903	15.122	2.309	33.545	1.00	20.56
660	N	TYR	A	904	19.742	-0.862	32.353	1.00	18.81
661	CA	TYR	A	904	20.025	-2.265	32.104	1.00	18.91
662	C	TYR	A	904	18.942	-3.146	32.731	1.00	18.72
663	O	TYR	A	904	18.572	-2.951	33.887	1.00	19.2
664	CB	TYR	A	904	21.39	-2.635	32.692	1.00	19.1
665	CG	TYR	A	904	21.679	-4.119	32.638	1.00	19.35
666	CD1	TYR	A	904	21.784	-4.781	31.415	1.00	19.43
667	CD2	TYR	A	904	21.812	-4.865	33.807	1.00	19.73
668	CE1	TYR	A	904	22.013	-6.155	31.356	1.00	19.84
669	CE2	TYR	A	904	22.045	-6.245	33.764	1.00	19.81
670	CZ	TYR	A	904	22.14	-6.88	32.536	1.00	19.9
671	OH	TYR	A	904	22.342	-8.238	32.481	1.00	20.31
672	N	ALA	A	905	18.441	-4.111	31.963	1.00	18.63
673	CA	ALA	A	905	17.406	-5.037	32.437	1.00	18.59
674	C	ALA	A	905	18.069	-6.378	32.752	1.00	18.27
675	O	ALA	A	905	18.37	-7.159	31.85	1.00	18.39
676	CB	ALA	A	905	16.323	-5.22	31.355	1.00	18.78
677	N	PRO	A	906	18.294	-6.665	34.04	1.00	18.07
678	CA	PRO	A	906	18.934	-7.912	34.48	1.00	18.03
679	C	PRO	A	906	18.211	-9.195	34.1	1.00	18.09



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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

680	O	PRO	A	906	18.83	-10.259	34.009	1.00	18.48
681	CB	PRO	A	906	19.018	-7.749	35.996	1.00	17.77
682	CG	PRO	A	906	19.007	-6.269	36.193	1.00	18.34
683	CD	PRO	A	906	18.003	-5.792	35.187	1.00	18.02
684	N	HIS	A	907	16.907	-9.103	33.867	1.00	17.71
685	CA	HIS	A	907	16.134	-10.29	33.538	1.00	17.47
686	C	HIS	A	907	15.729	-10.478	32.072	1.00	17.22
687	O	HIS	A	907	14.936	-11.366	31.759	1.00	17.06
688	CB	HIS	A	907	14.916	-10.332	34.454	1.00	17.58
689	CG	HIS	A	907	15.268	-10.237	35.906	1.00	17.69
690	ND1	HIS	A	907	15.961	-11.229	36.567	1.00	17.61
691	CD2	HIS	A	907	15.051	-9.258	36.817	1.00	17.96
692	CE1	HIS	A	907	16.155	-10.865	37.823	1.00	17.67
693	NE2	HIS	A	907	15.613	-9.673	38	1.00	17.85
694	N	GLY	A	908	16.277	-9.654	31.18	1.00	16.66
695	CA	GLY	A	908	15.968	-9.785	29.764	1.00	16.3
696	C	GLY	A	908	14.6	-9.289	29.328	1.00	16.15
697	O	GLY	A	908	13.919	-8.584	30.071	1.00	16.51
698	N	ASN	A	909	14.191	-9.654	28.117	1.00	15.53
699	CA	ASN	A	909	12.901	-9.217	27.614	1.00	15.46
700	C	ASN	A	909	11.765	-10.088	28.156	1.00	15.2
701	O	ASN	A	909	11.947	-11.279	28.432	1.00	14.78
702	CB	ASN	A	909	12.894	-9.203	26.075	1.00	15.69
703	CG	ASN	A	909	12.858	-10.596	25.471	1.00	16.45
704	OD1	ASN	A	909	11.854	-11.305	25.567	1.00	16.56
705	ND2	ASN	A	909	13.959	-10.995	24.841	1.00	16.72
706	N	LEU	A	910	10.593	-9.474	28.296	1.00	14.72
707	CA	LEU	A	910	9.413	-10.142	28.831	1.00	14.77
708	C	LEU	A	910	9.002	-11.44	28.137	1.00	14.94
709	O	LEU	A	910	8.562	-12.386	28.798	1.00	14.66
710	CB	LEU	A	910	8.228	-9.167	28.837	1.00	14.03
711	CG	LEU	A	910	6.883	-9.714	29.323	1.00	14.14
712	CD1	LEU	A	910	7.334	-10.316	30.715	1.00	13.73
713	CD2	LEU	A	910	5.848	-8.599	29.321	1.00	13.72
714	N	LEU	A	911	9.146	-11.494	26.816	1.00	15.17
715	CA	LEU	A	911	8.743	-12.685	26.084	1.00	15.78
716	C	LEU	A	911	9.525	-13.913	26.509	1.00	15.97
717	O	LEU	A	911	8.933	-14.944	26.815	1.00	15.89
718	CB	LEU	A	911	8.881	-12.475	24.571	1.00	15.75
719	CG	LEU	A	911	8.413	-13.662	23.707	1.00	15.94

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TABLE 4  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

720	CD1	LEU	A	911	6.969	-14.014	24.046	1.00	15.42
721	CD2	LEU	A	911	8.541	-13.313	22.216	1.00	15.71
722	N	ASP	A	912	10.85	-13.811	26.524	1.00	16.63
723	CA	ASP	A	912	11.671	-14.943	26.929	1.00	17.14
724	C	ASP	A	912	11.424	-15.275	28.385	1.00	16.76
725	O	ASP	A	912	11.383	-16.443	28.759	1.00	16.72
726	CB	ASP	A	912	13.166	-14.653	26.736	1.00	18.89
727	CG	ASP	A	912	13.583	-14.641	25.266	1.00	20.82
728	OD1	ASP	A	912	13.044	-15.457	24.482	1.00	22.31
729	OD2	ASP	A	912	14.462	-13.828	24.9	1.00	21.44
730	N	PHE	A	913	11.256	-14.245	29.207	1.00	16.47
731	CA	PHE	A	913	11.037	-14.458	30.629	1.00	16.45
732	C	PHE	A	913	9.769	-15.273	30.845	1.00	16.52
733	O	PHE	A	913	9.724	-16.165	31.696	1.00	16.21
734	CB	PHE	A	913	10.918	-13.119	31.353	1.00	16.57
735	CG	PHE	A	913	11.047	-13.225	32.848	1.00	16.54
736	CD1	PHE	A	913	12.29	-13.478	33.435	1.00	16.42
737	CD2	PHE	A	913	9.935	-13.066	33.67	1.00	16.1
738	CE1	PHE	A	913	12.419	-13.567	34.82	1.00	16.05
739	CE2	PHE	A	913	10.053	-13.152	35.056	1.00	16.36
740	CZ	PHE	A	913	11.299	-13.403	35.634	1.00	16.13
741	N	LEU	A	914	8.739	-14.952	30.067	1.00	16.36
742	CA	LEU	A	914	7.464	-15.651	30.153	1.00	16.24
743	C	LEU	A	914	7.612	-17.104	29.702	1.00	16.79
744	O	LEU	A	914	7.197	-18.028	30.4	1.00	16.72
745	CB	LEU	A	914	6.421	-14.948	29.282	1.00	15.4
746	CG	LEU	A	914	5.832	-13.648	29.826	1.00	14.89
747	CD1	LEU	A	914	5.049	-12.913	28.739	1.00	13.94
748	CD2	LEU	A	914	4.947	-13.977	31.023	1.00	14.12
749	N	ARG	A	915	8.206	-17.297	28.529	1.00	17.1
750	CA	ARG	A	915	8.388	-18.633	27.991	1.00	17.87
751	C	ARG	A	915	9.245	-19.506	28.902	1.00	18.38
752	O	ARG	A	915	8.962	-20.689	29.069	1.00	18.25
753	CB	ARG	A	915	8.98	-18.547	26.579	1.00	17.81
754	CG	ARG	A	915	7.987	-17.959	25.583	1.00	18.21
755	CD	ARG	A	915	8.531	-17.797	24.173	1.00	17.97
756	NE	ARG	A	915	7.45	-17.429	23.257	1.00	17.82
757	CZ	ARG	A	915	7.616	-17.102	21.977	1.00	17.98
758	NH1	ARG	A	915	6.562	-16.789	21.232	1.00	17.43
759	NH2	ARG	A	915	8.83	-17.079	21.444	1.00	17.99

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TABLE 4  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

760	N	LYS	A	916	10.27	-18.918	29.513	1.00	18.97
761	CA	LYS	A	916	11.137	-19.669	30.413	1.00	19.83
762	C	LYS	A	916	10.456	-20.027	31.739	1.00	19.77
763	O	LYS	A	916	11.026	-20.751	32.549	1.00	19.88
764	CB	LYS	A	916	12.421	-18.893	30.699	1.00	20.63
765	CG	LYS	A	916	13.352	-18.715	29.499	1.00	22.39
766	CD	LYS	A	916	14.637	-17.983	29.919	1.00	23.59
767	CE	LYS	A	916	15.507	-17.587	28.724	1.00	24.66
768	NZ	LYS	A	916	15.884	-18.742	27.847	1.00	25.37
769	N	SER	A	917	9.248	-19.527	31.974	1.00	19.77
770	CA	SER	A	917	8.558	-19.857	33.219	1.00	20.11
771	C	SER	A	917	7.691	-21.108	33.06	1.00	20.37
772	O	SER	A	917	7.124	-21.6	34.029	1.00	20.33
773	CB	SER	A	917	7.685	-18.686	33.693	1.00	19.87
774	OG	SER	A	917	6.514	-18.554	32.905	1.00	19.7
775	N	ARG	A	918	7.592	-21.616	31.835	1.00	21.21
776	CA	ARG	A	918	6.785	-22.804	31.558	1.00	22.36
777	C	ARG	A	918	7.487	-24.046	32.104	1.00	23.49
778	O	ARG	A	918	8.018	-24.855	31.343	1.00	23.52
779	CB	ARG	A	918	6.565	-22.95	30.05	1.00	21.41
780	CG	ARG	A	918	5.74	-21.837	29.436	1.00	21.13
781	CD	ARG	A	918	5.514	-22.076	27.963	1.00	20.61
782	NE	ARG	A	918	4.549	-21.135	27.406	1.00	20.53
783	CZ	ARG	A	918	3.959	-21.291	26.226	1.00	20.12
784	NH1	ARG	A	918	3.083	-20.392	25.788	1.00	19.17
785	NH2	ARG	A	918	4.244	-22.354	25.489	1.00	19.75
786	N	VAL	A	919	7.474	-24.181	33.427	1.00	24.86
787	CA	VAL	A	919	8.132	-25.286	34.11	1.00	26.57
788	C	VAL	A	919	7.659	-26.657	33.645	1.00	27.7
789	O	VAL	A	919	8.447	-27.597	33.572	1.00	28.07
790	CB	VAL	A	919	7.955	-25.168	35.648	1.00	26.64
791	CG1	VAL	A	919	6.477	-25.157	36.012	1.00	26.31
792	CG2	VAL	A	919	8.68	-26.316	36.346	1.00	26.85
793	N	LEU	A	920	6.375	-26.774	33.331	1.00	28.77
794	CA	LEU	A	920	5.841	-28.042	32.866	1.00	29.78
795	C	LEU	A	920	6.701	-28.555	31.715	1.00	30.49
796	O	LEU	A	920	7.014	-29.745	31.651	1.00	30.64
797	CB	LEU	A	920	4.388	-27.868	32.403	1.00	30
798	CG	LEU	A	920	3.658	-29.11	31.877	1.00	30
799	CD1	LEU	A	920	3.626	-30.183	32.954	1.00	29.9

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## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

800	CD2	LEU	A	920	2.236	-28.735	31.456	1.00	30.14
801	N	GLU	A	921	7.095	-27.648	30.82	1.00	31.22
802	CA	GLU	A	921	7.914	-28.008	29.662	1.00	31.9
803	C	GLU	A	921	9.401	-28.125	29.966	1.00	31.99
804	O	GLU	A	921	10.089	-28.968	29.388	1.00	31.99
805	CB	GLU	A	921	7.727	-26.997	28.523	1.00	32.53
806	CG	GLU	A	921	6.352	-27.032	27.886	1.00	34.15
807	CD	GLU	A	921	6.313	-26.431	26.486	1.00	35.27
808	OE1	GLU	A	921	6.563	-25.205	26.339	1.00	35.73
809	OE2	GLU	A	921	6.029	-27.196	25.532	1.00	35.42
810	N	THR	A	922	9.897	-27.284	30.867	1.00	31.97
811	CA	THR	A	922	11.313	-27.301	31.201	1.00	32.2
812	C	THR	A	922	11.683	-28.279	32.31	1.00	32.35
813	O	THR	A	922	12.803	-28.781	32.346	1.00	32.71
814	CB	THR	A	922	11.805	-25.892	31.602	1.00	32.16
815	OG1	THR	A	922	11.131	-25.463	32.791	1.00	31.78
816	CG2	THR	A	922	11.525	-24.895	30.476	1.00	32.08
817	N	ASP	A	923	10.745	-28.55	33.21	1.00	32.37
818	CA	ASP	A	923	10.997	-29.464	34.318	1.00	32.1
819	C	ASP	A	923	9.711	-30.193	34.71	1.00	31.82
820	O	ASP	A	923	9.149	-29.964	35.781	1.00	31.61
821	CB	ASP	A	923	11.546	-28.683	35.51	1.00	32.46
822	CG	ASP	A	923	12.068	-29.584	36.605	1.00	32.76
823	OD1	ASP	A	923	11.916	-30.816	36.486	1.00	33.12
824	OD2	ASP	A	923	12.629	-29.059	37.59	1.00	33.57
825	N	PRO	A	924	9.239	-31.099	33.842	1.00	31.88
826	CA	PRO	A	924	8.016	-31.879	34.06	1.00	31.81
827	C	PRO	A	924	7.9	-32.456	35.466	1.00	31.74
828	O	PRO	A	924	6.897	-32.252	36.158	1.00	31.61
829	CB	PRO	A	924	8.115	-32.97	32.997	1.00	31.87
830	CG	PRO	A	924	8.848	-32.292	31.894	1.00	31.8
831	CD	PRO	A	924	9.936	-31.558	32.627	1.00	31.73
832	N	ALA	A	925	8.934	-33.184	35.875	1.00	31.73
833	CA	ALA	A	925	8.972	-33.814	37.187	1.00	31.67
834	C	ALA	A	925	8.593	-32.83	38.279	1.00	31.67
835	O	ALA	A	925	7.766	-33.131	39.142	1.00	31.76
836	CB	ALA	A	925	10.358	-34.377	37.453	1.00	31.78
837	N	PHE	A	926	9.202	-31.652	38.24	1.00	31.48
838	CA	PHE	A	926	8.919	-30.63	39.233	1.00	31.44
839	C	PHE	A	926	7.502	-30.089	39.068	1.00	31.01

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TABLE 4

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

840	O	PHE	A	926	6.779	-29.897	40.046	1.00	30.83
841	CB	PHE	A	926	9.907	-29.474	39.108	1.00	31.94
842	CG	PHE	A	926	9.724	-28.427	40.157	1.00	32.45
843	CD1	PHE	A	926	10.08	-28.683	41.478	1.00	32.59
844	CD2	PHE	A	926	9.154	-27.198	39.839	1.00	32.67
845	CE1	PHE	A	926	9.869	-27.729	42.472	1.00	32.72
846	CE2	PHE	A	926	8.938	-26.238	40.824	1.00	32.75
847	CZ	PHE	A	926	9.297	-26.505	42.145	1.00	32.85
848	N	ALA	A	927	7.12	-29.834	37.822	1.00	30.56
849	CA	ALA	A	927	5.794	-29.316	37.522	1.00	30.17
850	C	ALA	A	927	4.696	-30.214	38.106	1.00	30
851	O	ALA	A	927	3.804	-29.741	38.807	1.00	29.47
852	CB	ALA	A	927	5.627	-29.193	36.02	1.00	29.86
853	N	ILE	A	928	4.781	-31.512	37.821	1.00	30.06
854	CA	ILE	A	928	3.798	-32.483	38.3	1.00	30.37
855	C	ILE	A	928	3.768	-32.575	39.822	1.00	30.29
856	O	ILE	A	928	2.709	-32.505	40.444	1.00	30.01
857	CB	ILE	A	928	4.095	-33.906	37.758	1.00	30.77
858	CG1	ILE	A	928	4.085	-33.908	36.228	1.00	30.97
859	CG2	ILE	A	928	3.076	-34.89	38.301	1.00	31
860	CD1	ILE	A	928	2.8	-33.422	35.628	1.00	31.2
861	N	ALA	A	929	4.948	-32.736	40.409	1.00	30.29
862	CA	ALA	A	929	5.086	-32.866	41.851	1.00	30.13
863	C	ALA	A	929	4.476	-31.706	42.619	1.00	29.91
864	O	ALA	A	929	3.981	-31.89	43.732	1.00	30.22
865	CB	ALA	A	929	6.564	-33.014	42.218	1.00	30.14
866	N	ASN	A	930	4.498	-30.514	42.032	1.00	29.47
867	CA	ASN	A	930	3.957	-29.348	42.715	1.00	28.8
868	C	ASN	A	930	2.725	-28.728	42.072	1.00	28.08
869	O	ASN	A	930	2.321	-27.622	42.426	1.00	27.89
870	CB	ASN	A	930	5.059	-28.309	42.873	1.00	29.68
871	CG	ASN	A	930	6.135	-28.764	43.836	1.00	30.2
872	OD1	ASN	A	930	5.996	-28.614	45.048	1.00	30.74
873	ND2	ASN	A	930	7.202	-29.352	43.303	1.00	30.46
874	N	SER	A	931	2.127	-29.456	41.138	1.00	27.42
875	CA	SER	A	931	0.924	-29.002	40.452	1.00	26.92
876	C	SER	A	931	1.008	-27.573	39.927	1.00	26.08
877	O	SER	A	931	0.046	-26.812	40.032	1.00	26.27
878	CB	SER	A	931	-0.277	-29.125	41.392	1.00	27.24
879	OG	SER	A	931	-0.43	-30.463	41.834	1.00	27.87

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

880	N	THR	A	932	2.152	-27.205	39.36	1.00	25.18
881	CA	THR	A	932	2.316	-25.861	38.82	1.00	24.39
882	C	THR	A	932	2.644	-25.873	37.336	1.00	23.5
883	O	THR	A	932	3.376	-26.74	36.859	1.00	23.38
884	CB	THR	A	932	3.428	-25.085	39.534	1.00	24.66
885	OG1	THR	A	932	3.553	-23.794	38.927	1.00	25.38
886	CG2	THR	A	932	4.757	-25.814	39.423	1.00	24.54
887	N	ALA	A	933	2.097	-24.905	36.608	1.00	22.49
888	CA	ALA	A	933	2.343	-24.803	35.178	1.00	21.55
889	C	ALA	A	933	3.268	-23.626	34.871	1.00	20.95
890	O	ALA	A	933	3.588	-23.369	33.714	1.00	20.35
891	CB	ALA	A	933	1.029	-24.643	34.435	1.00	21.63
892	N	SER	A	934	3.707	-22.924	35.913	1.00	20.3
893	CA	SER	A	934	4.589	-21.777	35.733	1.00	19.84
894	C	SER	A	934	5.29	-21.356	37.023	1.00	19.73
895	O	SER	A	934	4.756	-21.535	38.118	1.00	19.39
896	CB	SER	A	934	3.781	-20.592	35.188	1.00	19.6
897	OG	SER	A	934	4.576	-19.424	35.064	1.00	19.15
898	N	THR	A	935	6.487	-20.793	36.883	1.00	19.6
899	CA	THR	A	935	7.249	-20.305	38.034	1.00	19.56
900	C	THR	A	935	6.732	-18.921	38.41	1.00	19.49
901	O	THR	A	935	7.151	-18.334	39.406	1.00	19.62
902	CB	THR	A	935	8.747	-20.175	37.711	1.00	19.68
903	OG1	THR	A	935	8.915	-19.334	36.562	1.00	19.41
904	CG2	THR	A	935	9.355	-21.546	37.441	1.00	19.7
905	N	LEU	A	936	5.829	-18.394	37.592	1.00	19.2
906	CA	LEU	A	936	5.251	-17.085	37.848	1.00	19.06
907	C	LEU	A	936	3.848	-17.26	38.416	1.00	19.11
908	O	LEU	A	936	3.165	-18.232	38.109	1.00	19.03
909	CB	LEU	A	936	5.195	-16.272	36.55	1.00	19.04
910	CG	LEU	A	936	6.549	-15.964	35.902	1.00	18.91
911	CD1	LEU	A	936	6.336	-15.254	34.57	1.00	18.38
912	CD2	LEU	A	936	7.386	-15.107	36.851	1.00	18.99
913	N	SER	A	937	3.427	-16.323	39.256	1.00	19.33
914	CA	SER	A	937	2.099	-16.386	39.856	1.00	19.39
915	C	SER	A	937	1.163	-15.426	39.14	1.00	19.18
916	O	SER	A	937	1.608	-14.54	38.411	1.00	19.21
917	CB	SER	A	937	2.162	-16.016	41.346	1.00	19.77
918	OG	SER	A	937	2.596	-14.674	41.542	1.00	19.94
919	N	SER	A	938	-0.134	-15.615	39.348	1.00	18.92

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

920	CA	SER	A	938	-1.139	-14.747	38.755	1.00	18.79
921	C	SER	A	938	-0.817	-13.283	39.072	1.00	18.91
922	O	SER	A	938	-0.882	-12.431	38.188	1.00	19.02
923	CB	SER	A	938	-2.526	-15.101	39.305	1.00	18.4
924	OG	SER	A	938	-3.521	-14.204	38.838	1.00	17.51
925	N	GLN	A	939	-0.467	-13.002	40.33	1.00	19.04
926	CA	GLN	A	939	-0.139	-11.64	40.765	1.00	19.26
927	C	GLN	A	939	1.06	-11.024	40.056	1.00	18.55
928	O	GLN	A	939	1.02	-9.854	39.698	1.00	18.05
929	CB	GLN	A	939	0.113	-11.588	42.28	1.00	20.35
930	CG	GLN	A	939	-1.142	-11.63	43.156	1.00	22.64
931	CD	GLN	A	939	-2.043	-10.41	42.986	1.00	23.31
932	OE1	GLN	A	939	-2.884	-10.368	42.086	1.00	24.69
933	NE2	GLN	A	939	-1.865	-9.411	43.849	1.00	23.28
934	N	GLN	A	940	2.13	-11.798	39.876	1.00	18.06
935	CA	GLN	A	940	3.321	-11.295	39.194	1.00	17.77
936	C	GLN	A	940	2.968	-10.995	37.741	1.00	16.92
937	O	GLN	A	940	3.424	-10.008	37.166	1.00	16.44
938	CB	GLN	A	940	4.46	-12.327	39.239	1.00	18.48
939	CG	GLN	A	940	5.066	-12.541	40.622	1.00	19.68
940	CD	GLN	A	940	6.068	-13.693	40.653	1.00	20.48
941	OE1	GLN	A	940	5.699	-14.866	40.504	1.00	20.27
942	NE2	GLN	A	940	7.343	-13.36	40.84	1.00	20.86
943	N	LEU	A	941	2.151	-11.86	37.153	1.00	16.36
944	CA	LEU	A	941	1.736	-11.679	35.766	1.00	15.78
945	C	LEU	A	941	0.923	-10.395	35.633	1.00	15.38
946	O	LEU	A	941	1.151	-9.612	34.712	1.00	15.27
947	CB	LEU	A	941	0.934	-12.895	35.291	1.00	15.01
948	CG	LEU	A	941	1.779	-14.174	35.18	1.00	14.88
949	CD1	LEU	A	941	0.876	-15.369	34.912	1.00	14.66
950	CD2	LEU	A	941	2.823	-14.02	34.06	1.00	13.95
951	N	LEU	A	942	0.001	-10.164	36.567	1.00	15.41
952	CA	LEU	A	942	-0.313	-8.954	36.533	1.00	15.95
953	C	LEU	A	942	0.04	-7.702	36.759	1.00	16
954	O	LEU	A	942	-0.267	-6.628	36.226	1.00	16.08
955	CB	LEU	A	942	-1.931	-9.014	37.58	1.00	16.41
956	CG	LEU	A	942	-3.097	-9.991	37.363	1.00	17.09
957	CD1	LEU	A	942	-4.14	-9.777	38.447	1.00	17.3
958	CD2	LEU	A	942	-3.729	-9.77	35.998	1.00	17.31
959	N	HIS	A	943	1.106	-7.835	37.548	1.00	15.69

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

960	CA	HIS	A	943	1.994	-6.705	37.805	1.00	15.8
961	C	HIS	A	943	2.694	-6.285	36.508	1.00	15.07
962	O	HIS	A	943	2.831	-5.094	36.223	1.00	14.96
963	CB	HIS	A	943	3.033	-7.062	38.88	1.00	16.95
964	CG	HIS	A	943	2.576	-6.776	40.277	1.00	18.5
965	ND1	HIS	A	943	2.206	-5.514	40.693	1.00	19.31
966	CD2	HIS	A	943	2.435	-7.584	41.357	1.00	19.02
967	CE1	HIS	A	943	1.858	-5.556	41.968	1.00	19.59
968	NE2	HIS	A	943	1.987	-6.801	42.395	1.00	19.61
969	N	PHE	A	944	3.142	-7.262	35.728	1.00	14.36
970	CA	PHE	A	944	3.799	-6.966	34.458	1.00	14.06
971	C	PHE	A	944	2.83	-6.163	33.603	1.00	13.57
972	O	PHE	A	944	3.192	-5.149	33.01	1.00	12.99
973	CB	PHE	A	944	4.155	-8.26	33.715	1.00	14.86
974	CG	PHE	A	944	5.338	-8.992	34.284	1.00	15.15
975	CD1	PHE	A	944	5.422	-10.373	34.184	1.00	15.56
976	CD2	PHE	A	944	6.383	-8.301	34.887	1.00	15.95
977	CE1	PHE	A	944	6.533	-11.064	34.677	1.00	16.3
978	CE2	PHE	A	944	7.502	-8.979	35.384	1.00	16.16
979	CZ	PHE	A	944	7.574	-10.361	35.277	1.00	16.35
980	N	ALA	A	945	1.59	-6.637	33.542	1.00	13.09
981	CA	ALA	A	945	0.564	-5.97	32.755	1.00	13.03
982	C	ALA	A	945	0.317	-4.553	33.259	1.00	12.78
983	O	ALA	A	945	0.281	-3.615	32.473	1.00	12.32
984	CB	ALA	A	945	-0.731	-6.78	32.788	1.00	12.8
985	N	ALA	A	946	0.159	-4.403	34.57	1.00	12.85
986	CA	ALA	A	946	-0.08	-3.091	35.168	1.00	13.06
987	C	ALA	A	946	1.096	-2.16	34.92	1.00	13.12
988	O	ALA	A	946	0.908	-0.983	34.618	1.00	13.28
989	CB	ALA	A	946	-0.333	-3.234	36.678	1.00	12.97
990	N	ASP	A	947	2.312	-2.687	35.05	1.00	13.43
991	CA	ASP	A	947	3.518	-1.892	34.818	1.00	13.31
992	C	ASP	A	947	3.512	-1.276	33.416	1.00	13.16
993	O	ASP	A	947	3.772	-0.078	33.247	1.00	12.98
994	CB	ASP	A	947	4.772	-2.759	34.951	1.00	14.3
995	CG	ASP	A	947	5.237	-2.933	36.391	1.00	15.18
996	OD1	ASP	A	947	6.228	-3.672	36.585	1.00	15.8
997	OD2	ASP	A	947	4.635	-2.341	37.317	1.00	15.64
998	N	VAL	A	948	3.235	-2.103	32.41	1.00	12.5
999	CA	VAL	A	948	3.223	-1.623	31.032	1.00	12.48



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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

1000	C	VAL	A	948	2.103	-0.61	30.833	1.00	12.55
1001	O	VAL	A	948	2.284	0.389	30.144	1.00	12.58
1002	CB	VAL	A	948	3.057	-2.782	30.024	1.00	12.11
1003	CG1	VAL	A	948	2.978	-2.234	28.589	1.00	11.8
1004	CG2	VAL	A	948	4.234	-3.73	30.142	1.00	12.11
1005	N	ALA	A	949	0.956	-0.861	31.455	1.00	12.48
1006	CA	ALA	A	949	-0.173	0.055	31.338	1.00	12.82
1007	C	ALA	A	949	0.212	1.429	31.894	1.00	12.89
1008	O	ALA	A	949	-0.034	2.465	31.264	1.00	12.55
1009	CB	ALA	A	949	-1.378	-0.5	32.092	1.00	12.42
1010	N	ARG	A	950	0.819	1.427	33.077	1.00	13.29
1011	CA	ARG	A	950	1.233	2.664	33.725	1.00	13.66
1012	C	ARG	A	950	2.271	3.346	32.839	1.00	14.07
1013	O	ARG	A	950	2.243	4.563	32.647	1.00	13.85
1014	CB	ARG	A	950	1.831	2.361	35.103	1.00	13.76
1015	CG	ARG	A	950	2.131	3.591	35.948	1.00	13.85
1016	CD	ARG	A	950	2.766	3.217	37.298	1.00	14.76
1017	NE	ARG	A	950	1.979	2.224	38.032	1.00	15.36
1018	CZ	ARG	A	950	2.289	0.932	38.124	1.00	15.91
1019	NH1	ARG	A	950	1.508	0.108	38.81	1.00	15.73
1020	NH2	ARG	A	950	3.389	0.462	37.541	1.00	16.65
1021	N	GLY	A	951	3.181	2.545	32.296	1.00	14.14
1022	CA	GLY	A	951	4.21	3.087	31.432	1.00	14.89
1023	C	GLY	A	951	3.618	3.728	30.191	1.00	15.31
1024	O	GLY	A	951	4.047	4.809	29.779	1.00	15.18
1025	N	MET	A	952	2.631	3.065	29.589	1.00	15.19
1026	CA	MET	A	952	1.997	3.597	28.393	1.00	15.44
1027	C	MET	A	952	1.105	4.791	28.703	1.00	15.49
1028	O	MET	A	952	0.917	5.668	27.86	1.00	15.9
1029	CB	MET	A	952	1.197	2.507	27.678	1.00	15.61
1030	CG	MET	A	952	2.066	1.507	26.912	1.00	15.82
1031	SD	MET	A	952	3.249	2.321	25.801	1.00	16.89
1032	CE	MET	A	952	2.181	3.353	24.801	1.00	16.72
1033	N	ASP	A	953	0.557	4.833	29.911	1.00	15.68
1034	CA	ASP	A	953	-0.283	5.956	30.306	1.00	15.84
1035	C	ASP	A	953	0.607	7.194	30.332	1.00	15.72
1036	O	ASP	A	953	0.24	8.258	29.825	1.00	15.39
1037	CB	ASP	A	953	-0.89	5.708	31.693	1.00	16.32
1038	CG	ASP	A	953	-1.714	6.89	32.199	1.00	17.35
1039	OD1	ASP	A	953	-2.479	7.478	31.408	1.00	17.42

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

1040	OD2	ASP	A	953	-1.605	7.224	33.399	1.00	18.45
1041	N	TYR	A	954	1.786	7.037	30.923	1.00	15.66
1042	CA	TYR	A	954	2.753	8.121	31.018	1.00	16.02
1043	C	TYR	A	954	3.152	8.607	29.625	1.00	16.24
1044	O	TYR	A	954	3.05	9.791	29.317	1.00	16.03
1045	CB	TYR	A	954	3.999	7.64	31.765	1.00	16.05
1046	CG	TYR	A	954	5.147	8.623	31.743	1.00	16.15
1047	CD1	TYR	A	954	5.156	9.742	32.585	1.00	16.23
1048	CD2	TYR	A	954	6.225	8.436	30.878	1.00	16
1049	CE1	TYR	A	954	6.216	10.653	32.566	1.00	16.04
1050	CE2	TYR	A	954	7.285	9.335	30.847	1.00	16.49
1051	CZ	TYR	A	954	7.277	10.442	31.696	1.00	16.44
1052	OH	TYR	A	954	8.333	11.32	31.67	1.00	16.67
1053	N	LEU	A	955	3.598	7.679	28.786	1.00	16.58
1054	CA	LEU	A	955	4.027	8.01	27.432	1.00	17.18
1055	C	LEU	A	955	2.93	8.611	26.546	1.00	17.55
1056	O	LEU	A	955	3.154	9.624	25.879	1.00	17.33
1057	CB	LEU	A	955	4.613	6.768	26.748	1.00	17.15
1058	CG	LEU	A	955	5.947	6.252	27.312	1.00	17.67
1059	CD1	LEU	A	955	6.391	4.992	26.557	1.00	17.29
1060	CD2	LEU	A	955	7.002	7.344	27.183	1.00	17.07
1061	N	SER	A	956	1.755	7.99	26.524	1.00	18.03
1062	CA	SER	A	956	0.673	8.499	25.691	1.00	18.92
1063	C	SER	A	956	0.243	9.887	26.15	1.00	19.72
1064	O	SER	A	956	-0.137	10.724	25.336	1.00	19.62
1065	CB	SER	A	956	-0.521	7.544	25.707	1.00	18.36
1066	OG	SER	A	956	-0.994	7.349	27.02	1.00	18.65
1067	N	GLN	A	957	0.32	10.135	27.453	1.00	21.01
1068	CA	GLN	A	957	-0.062	11.44	27.986	1.00	22.29
1069	C	GLN	A	957	0.919	12.485	27.469	1.00	22.3
1070	O	GLN	A	957	0.601	13.668	27.402	1.00	22.49
1071	CB	GLN	A	957	-0.052	11.426	29.516	1.00	23.49
1072	CG	GLN	A	957	-0.953	12.477	30.135	1.00	25.87
1073	CD	GLN	A	957	-2.193	11.886	30.803	1.00	27.05
1074	OE1	GLN	A	957	-3.236	12.544	30.895	1.00	28.04
1075	NE2	GLN	A	957	-2.079	10.653	31.288	1.00	27.3
1076	N	LYS	A	958	2.118	12.046	27.103	1.00	22.26
1077	CA	LYS	A	958	3.107	12.968	26.567	1.00	22.41
1078	C	LYS	A	958	3.118	12.949	25.036	1.00	22.13
1079	O	LYS	A	958	4.042	13.454	24.4	1.00	21.75

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

1080	CB	LYS	A	958	4.496	12.656	27.139	1.00	23.1
1081	CG	LYS	A	958	4.571	12.925	28.641	1.00	23.97
1082	CD	LYS	A	958	5.971	13.321	29.102	1.00	24.9
1083	CE	LYS	A	958	5.932	13.835	30.546	1.00	25.61
1084	NZ	LYS	A	958	7.19	14.526	30.954	1.00	25.84
1085	N	GLN	A	959	2.072	12.358	24.46	1.00	21.98
1086	CA	GLN	A	959	1.899	12.285	23.015	1.00	21.89
1087	C	GLN	A	959	2.732	11.266	22.252	1.00	21.28
1088	O	GLN	A	959	2.825	11.348	21.034	1.00	21.48
1089	CB	GLN	A	959	2.124	13.671	22.399	1.00	22.82
1090	CG	GLN	A	959	1.086	14.694	22.818	1.00	24.1
1091	CD	GLN	A	959	-0.29	14.331	22.315	1.00	24.88
1092	OE1	GLN	A	959	-0.505	14.211	21.108	1.00	25.48
1093	NE2	GLN	A	959	-1.235	14.147	23.235	1.00	25.72
1094	N	PHE	A	960	3.344	10.311	22.942	1.00	20.65
1095	CA	PHE	A	960	4.137	9.309	22.239	1.00	19.68
1096	C	PHE	A	960	3.24	8.218	21.691	1.00	18.92
1097	O	PHE	A	960	2.214	7.89	22.281	1.00	18.36
1098	CB	PHE	A	960	5.171	8.648	23.16	1.00	20.28
1099	CG	PHE	A	960	6.362	9.512	23.478	1.00	20.91
1100	CD1	PHE	A	960	6.295	10.476	24.475	1.00	21.09
1101	CD2	PHE	A	960	7.557	9.348	22.785	1.00	21.4
1102	CE1	PHE	A	960	7.4	11.265	24.784	1.00	21.64
1103	CE2	PHE	A	960	8.675	10.134	23.083	1.00	21.75
1104	CZ	PHE	A	960	8.596	11.095	24.087	1.00	21.7
1105	N	ILE	A	961	3.629	7.681	20.54	1.00	18.16
1106	CA	ILE	A	961	2.923	6.575	19.914	1.00	17.47
1107	C	ILE	A	961	4.013	5.517	19.774	1.00	17.08
1108	O	ILE	A	961	5.009	5.731	19.08	1.00	16.28
1109	CB	ILE	A	961	2.366	6.952	18.523	1.00	17.3
1110	CG1	ILE	A	961	1.352	8.093	18.666	1.00	17.24
1111	CG2	ILE	A	961	1.699	5.726	17.878	1.00	16.79
1112	CD1	ILE	A	961	0.838	8.64	17.345	1.00	16.82
1113	N	HIS	A	962	3.832	4.382	20.442	1.00	16.81
1114	CA	HIS	A	962	4.84	3.331	20.405	1.00	16.65
1115	C	HIS	A	962	4.964	2.591	19.071	1.00	16.92
1116	O	HIS	A	962	6.072	2.409	18.569	1.00	16.82
1117	CB	HIS	A	962	4.594	2.338	21.54	1.00	16.48
1118	CG	HIS	A	962	5.733	1.389	21.756	1.00	16.63
1119	ND1	HIS	A	962	6.047	0.389	20.861	1.00	16.5

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

1120	CD2	HIS	A	962	6.673	1.333	22.729	1.00	16.58
1121	CE1	HIS	A	962	7.134	-0.24	21.272	1.00	16.95
1122	NE2	HIS	A	962	7.534	0.314	22.403	1.00	16.68
1123	N	ARG	A	963	3.832	2.166	18.51	1.00	17.07
1124	CA	ARG	A	963	3.778	1.455	17.226	1.00	17.5
1125	C	ARG	A	963	4.166	-0.03	17.234	1.00	17.26
1126	O	ARG	A	963	3.845	-0.756	16.293	1.00	16.87
1127	CB	ARG	A	963	4.66	2.133	16.173	1.00	18.64
1128	CG	ARG	A	963	4.439	3.619	15.943	1.00	20.41
1129	CD	ARG	A	963	5.133	4.042	14.643	1.00	21.54
1130	NE	ARG	A	963	6.448	3.41	14.498	1.00	23.13
1131	CZ	ARG	A	963	7.532	3.752	15.192	1.00	24.16
1132	NH1	ARG	A	963	7.47	4.731	16.082	1.00	24.76
1133	NH2	ARG	A	963	8.679	3.104	15.01	1.00	24.65
1134	N	ASP	A	964	4.851	-0.494	18.273	1.00	16.82
1135	CA	ASP	A	964	5.269	-1.887	18.281	1.00	16.46
1136	C	ASP	A	964	5.202	-2.52	19.663	1.00	16.1
1137	O	ASP	A	964	6.131	-3.192	20.103	1.00	15.74
1138	CB	ASP	A	964	6.688	-1.985	17.709	1.00	16.82
1139	CG	ASP	A	964	7.063	-3.395	17.31	1.00	17.22
1140	OD1	ASP	A	964	6.161	-4.247	17.195	1.00	17.47
1141	OD2	ASP	A	964	8.268	-3.648	17.096	1.00	18.42
1142	N	LEU	A	965	4.088	-2.299	20.342	1.00	15.38
1143	CA	LEU	A	965	3.893	-2.843	21.668	1.00	14.92
1144	C	LEU	A	965	3.766	-4.361	21.565	1.00	14.73
1145	O	LEU	A	965	2.949	-4.876	20.791	1.00	14.65
1146	CB	LEU	A	965	2.63	-2.241	22.278	1.00	14.89
1147	CG	LEU	A	965	2.699	-1.626	23.669	1.00	15.35
1148	CD1	LEU	A	965	4.035	-0.915	23.897	1.00	14.8
1149	CD2	LEU	A	965	1.527	-0.663	23.817	1.00	14.95
1150	N	ALA	A	966	4.595	-5.064	22.334	1.00	13.97
1151	CA	ALA	A	966	4.612	-6.528	22.366	1.00	13.34
1152	C	ALA	A	966	5.557	-6.943	23.483	1.00	12.97
1153	O	ALA	A	966	6.387	-6.146	23.927	1.00	12.89
1154	CB	ALA	A	966	5.1	-7.089	21.033	1.00	12.8
1155	N	ALA	A	967	5.433	-8.185	23.934	1.00	12.7
1156	CA	ALA	A	967	6.269	-8.691	25.014	1.00	12.82
1157	C	ALA	A	967	7.765	-8.581	24.691	1.00	13.04
1158	O	ALA	A	967	8.576	-8.317	25.577	1.00	12.56
1159	CB	ALA	A	967	5.896	-10.136	25.316	1.00	12.82

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

1160	N	ARG	A	968	8.119	-8.776	23.424	1.00	13.21
1161	CA	ARG	A	968	9.512	-8.693	22.996	1.00	14.24
1162	C	ARG	A	968	10.059	-7.281	23.177	1.00	14.52
1163	O	ARG	A	968	11.275	-7.075	23.182	1.00	14.48
1164	CB	ARG	A	968	9.646	-9.09	21.525	1.00	14.47
1165	CG	ARG	A	968	8.785	-8.256	20.592	1.00	15.09
1166	CD	ARG	A	968	9.155	-8.48	19.115	1.00	16.04
1167	NE	ARG	A	968	8.313	-7.668	18.243	1.00	16.55
1168	CZ	ARG	A	968	7.049	-7.952	17.945	1.00	17.24
1169	NH1	ARG	A	968	6.469	-9.042	18.439	1.00	17.58
1170	NH2	ARG	A	968	6.356	-7.133	17.171	1.00	17.94
1171	N	ASN	A	969	9.162	-6.307	23.301	1.00	14.56
1172	CA	ASN	A	969	9.584	-4.932	23.485	1.00	14.86
1173	C	ASN	A	969	9.405	-4.442	24.909	1.00	14.61
1174	O	ASN	A	969	9.415	-3.243	25.18	1.00	14.84
1175	CB	ASN	A	969	8.869	-4.013	22.497	1.00	15.48
1176	CG	ASN	A	969	9.587	-3.954	21.162	1.00	16.45
1177	OD1	ASN	A	969	10.82	-4.032	21.12	1.00	16.57
1178	ND2	ASN	A	969	8.836	-3.805	20.072	1.00	16.29
1179	N	ILE	A	970	9.236	-5.388	25.82	1.00	14.33
1180	CA	ILE	A	970	9.106	-5.069	27.227	1.00	13.99
1181	C	ILE	A	970	10.278	-5.761	27.901	1.00	14.3
1182	O	ILE	A	970	10.59	-6.911	27.594	1.00	14.39
1183	CB	ILE	A	970	7.785	-5.602	27.831	1.00	13.43
1184	CG1	ILE	A	970	6.584	-5.059	27.049	1.00	12.49
1185	CG2	ILE	A	970	7.696	-5.198	29.3	1.00	12.83
1186	CD1	ILE	A	970	6.496	-3.537	26.997	1.00	11.57
1187	N	LEU	A	971	10.943	-5.052	28.803	1.00	14.8
1188	CA	LEU	A	971	12.08	-5.611	29.507	1.00	15.17
1189	C	LEU	A	971	11.783	-5.767	30.988	1.00	15.52
1190	O	LEU	A	971	11.087	-4.947	31.58	1.00	15.41
1191	CB	LEU	A	971	13.298	-4.712	29.284	1.00	15.45
1192	CG	LEU	A	971	13.663	-4.711	27.793	1.00	15.78
1193	CD1	LEU	A	971	14.074	-3.335	27.339	1.00	16.11
1194	CD2	LEU	A	971	14.738	-5.736	27.539	1.00	15.39
1195	N	VAL	A	972	12.291	-6.841	31.578	1.00	15.94
1196	CA	VAL	A	972	12.091	-7.084	32.998	1.00	16.75
1197	C	VAL	A	972	13.327	-6.53	33.708	1.00	17.48
1198	O	VAL	A	972	14.401	-7.144	33.691	1.00	17.18
1199	CB	VAL	A	972	11.94	-8.594	33.29	1.00	16.77

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TABLE 4  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

1200	CG1	VAL	A	972	11.527	-8.809	34.736	1.00	16.6
1201	CG2	VAL	A	972	10.912	-9.196	32.351	1.00	16.59
1202	N	GLY	A	973	13.174	-5.353	34.308	1.00	18.01
1203	CA	GLY	A	973	14.29	-4.722	34.987	1.00	19.24
1204	C	GLY	A	973	14.459	-5.145	36.43	1.00	20.13
1205	O	GLY	A	973	13.963	-6.198	36.837	1.00	20.28
1206	N	GLU	A	974	15.164	-4.317	37.197	1.00	21.07
1207	CA	GLU	A	974	15.425	-4.567	38.613	1.00	22.08
1208	C	GLU	A	974	14.141	-4.767	39.401	1.00	22.18
1209	O	GLU	A	974	13.156	-4.056	39.185	1.00	21.99
1210	CB	GLU	A	974	16.208	-3.391	39.209	1.00	23.17
1211	CG	GLU	A	974	17.682	-3.379	38.838	1.00	25.3
1212	CD	GLU	A	974	18.377	-2.074	39.199	1.00	26.57
1213	OE1	GLU	A	974	18.228	-1.592	40.348	1.00	27.36
1214	OE2	GLU	A	974	19.084	-1.531	38.327	1.00	27.61
1215	N	ASN	A	975	14.157	-5.729	40.319	1.00	22.2
1216	CA	ASN	A	975	12.985	-6.021	41.146	1.00	22.4
1217	C	ASN	A	975	11.816	-6.477	40.277	1.00	21.91
1218	O	ASN	A	975	10.657	-6.355	40.672	1.00	21.61
1219	CB	ASN	A	975	12.567	-4.777	41.938	1.00	23.51
1220	CG	ASN	A	975	13.589	-4.371	42.985	1.00	24.87
1221	OD1	ASN	A	975	13.707	-3.189	43.325	1.00	25.64
1222	ND2	ASN	A	975	14.321	-5.348	43.519	1.00	25.56
1223	N	TYR	A	976	12.136	-6.986	39.09	1.00	21.2
1224	CA	TYR	A	976	11.141	-7.469	38.138	1.00	20.68
1225	C	TYR	A	976	10.125	-6.424	37.683	1.00	19.92
1226	O	TYR	A	976	9.004	-6.768	37.309	1.00	19.65
1227	CB	TYR	A	976	10.407	-8.69	38.704	1.00	21.43
1228	CG	TYR	A	976	11.344	-9.802	39.098	1.00	22.34
1229	CD1	TYR	A	976	12.025	-9.766	40.316	1.00	23.02
1230	CD2	TYR	A	976	11.606	-10.856	38.228	1.00	22.69
1231	CE1	TYR	A	976	12.952	-10.753	40.658	1.00	23.41
1232	CE2	TYR	A	976	12.531	-11.848	38.555	1.00	23.38
1233	CZ	TYR	A	976	13.204	-11.788	39.775	1.00	23.64
1234	OH	TYR	A	976	14.137	-12.751	40.1	1.00	23.78
1235	N	VAL	A	977	10.516	-5.153	37.723	1.00	18.95
1236	CA	VAL	A	977	9.648	-4.063	37.272	1.00	18.21
1237	C	VAL	A	977	9.712	-4.051	35.743	1.00	17.7
1238	O	VAL	A	977	10.799	-4.007	35.166	1.00	17.79
1239	CB	VAL	A	977	10.137	-2.686	37.799	1.00	18.12

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TABLE 4

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

1240	CG1	VAL	A	977	9.35	-1.557	37.14	1.00	18.51
1241	CG2	VAL	A	977	9.966	-2.618	39.303	1.00	18.23
1242	N	ALA	A	978	8.556	-4.106	35.088	1.00	17.09
1243	CA	ALA	A	978	8.506	-4.104	33.63	1.00	16.03
1244	C	ALA	A	978	8.789	-2.708	33.068	1.00	15.86
1245	O	ALA	A	978	8.273	-1.7	33.566	1.00	15.33
1246	CB	ALA	A	978	7.146	-4.603	33.152	1.00	16.17
1247	N	LYS	A	979	9.616	-2.659	32.028	1.00	15.4
1248	CA	LYS	A	979	9.985	-1.398	31.399	1.00	15.55
1249	C	LYS	A	979	9.835	-1.478	29.888	1.00	15.25
1250	O	LYS	A	979	10.267	-2.44	29.259	1.00	14.93
1251	CB	LYS	A	979	11.426	-1.031	31.772	1.00	16.17
1252	CG	LYS	A	979	11.603	-0.696	33.257	1.00	16.76
1253	CD	LYS	A	979	13.071	-0.573	33.642	1.00	17.26
1254	CE	LYS	A	979	13.221	-0.028	35.059	1.00	17.85
1255	NZ	LYS	A	979	12.813	1.414	35.135	1.00	18.37
1256	N	ILE	A	980	9.215	-0.452	29.318	1.00	14.9
1257	CA	ILE	A	980	8.974	-0.389	27.883	1.00	14.75
1258	C	ILE	A	980	10.185	0.115	27.098	1.00	15.26
1259	O	ILE	A	980	10.713	1.194	27.385	1.00	14.71
1260	CB	ILE	A	980	7.785	0.557	27.575	1.00	14.55
1261	CG1	ILE	A	980	6.549	0.136	28.379	1.00	14.33
1262	CG2	ILE	A	980	7.489	0.555	26.08	1.00	14.4
1263	CD1	ILE	A	980	5.464	1.215	28.445	1.00	14.59
1264	N	ALA	A	981	10.625	-0.669	26.117	1.00	15.89
1265	CA	ALA	A	981	11.737	-0.251	25.27	1.00	16.97
1266	C	ALA	A	981	11.154	0.951	24.527	1.00	17.6
1267	O	ALA	A	981	10.12	0.843	23.871	1.00	17.75
1268	CB	ALA	A	981	12.121	-1.367	24.289	1.00	16.72
1269	N	ASP	A	982	11.823	2.09	24.63	1.00	18.61
1270	CA	ASP	A	982	11.324	3.328	24.047	1.00	19.52
1271	C	ASP	A	982	12.232	4.009	23.025	1.00	20.05
1272	O	ASP	A	982	12.371	5.232	23.037	1.00	19.88
1273	CB	ASP	A	982	11.028	4.29	25.195	1.00	19.8
1274	CG	ASP	A	982	12.162	4.337	26.219	1.00	20.46
1275	OD1	ASP	A	982	11.945	4.848	27.34	1.00	21.02
1276	OD2	ASP	A	982	13.276	3.866	25.899	1.00	20.19
1277	N	PHE	A	983	12.833	3.227	22.136	1.00	20.64
1278	CA	PHE	A	983	13.717	3.787	21.118	1.00	21.55
1279	C	PHE	A	983	13	3.897	19.776	1.00	21.98

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TABLE 4  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

1280	O	PHE	A	983	12.358	2.95	19.337	1.00	22.13
1281	CB	PHE	A	983	14.963	2.913	20.947	1.00	21.54
1282	CG	PHE	A	983	15.969	3.481	19.987	1.00	21.58
1283	CD1	PHE	A	983	16.745	4.581	20.346	1.00	21.61
1284	CD2	PHE	A	983	16.115	2.942	18.713	1.00	21.6
1285	CE1	PHE	A	983	17.652	5.142	19.448	1.00	21.83
1286	CE2	PHE	A	983	17.015	3.489	17.806	1.00	21.88
1287	CZ	PHE	A	983	17.789	4.594	18.171	1.00	21.9
1288	N	GLY	A	984	13.117	5.054	19.133	1.00	22.7
1289	CA	GLY	A	984	12.485	5.254	17.841	1.00	23.64
1290	C	GLY	A	984	10.974	5.374	17.888	1.00	24.14
1291	O	GLY	A	984	10.286	4.917	16.977	1.00	24.85
1292	N	LEU	A	985	10.445	5.989	18.941	1.00	24.2
1293	CA	LEU	A	985	9	6.147	19.064	1.00	23.89
1294	C	LEU	A	985	8.516	7.386	18.324	1.00	23.88
1295	O	LEU	A	985	9.293	8.3	18.049	1.00	23.91
1296	CB	LEU	A	985	8.594	6.244	20.54	1.00	23.52
1297	CG	LEU	A	985	9.043	5.111	21.468	1.00	23.56
1298	CD1	LEU	A	985	8.234	5.172	22.755	1.00	23.17
1299	CD2	LEU	A	985	8.848	3.753	20.79	1.00	23.31
1300	N	SER	A	986	7.228	7.414	18.004	1.00	23.95
1301	CA	SER	A	986	6.642	8.552	17.308	1.00	23.92
1302	C	SER	A	986	5.96	9.469	18.313	1.00	24.18
1303	O	SER	A	986	5.721	9.084	19.459	1.00	23.74
1304	CB	SER	A	986	5.627	8.076	16.271	1.00	23.82
1305	OG	SER	A	986	6.252	7.265	15.292	1.00	23.81
1306	N	ARG	A	987	5.639	10.681	17.878	1.00	24.49
1307	CA	ARG	A	987	4.996	11.637	18.757	1.00	25.1
1308	C	ARG	A	987	3.96	12.456	17.986	1.00	24.82
1309	O	ARG	A	987	4.266	13.02	16.941	1.00	25.19
1310	CB	ARG	A	987	6.069	12.543	19.356	1.00	26.22
1311	CG	ARG	A	987	5.645	13.305	20.576	1.00	27.44
1312	CD	ARG	A	987	6.775	13.312	21.589	1.00	28.87
1313	NE	ARG	A	987	6.536	14.281	22.65	1.00	30.07
1314	CZ	ARG	A	987	6.575	15.596	22.475	1.00	30.74
1315	NH1	ARG	A	987	6.849	16.098	21.275	1.00	30.91
1316	NH2	ARG	A	987	6.337	16.41	23.498	1.00	31.23
1317	N	GLY	A	988	2.736	12.507	18.5	1.00	24.3
1318	CA	GLY	A	988	1.677	13.252	17.838	1.00	23.78
1319	C	GLY	A	988	0.341	12.553	18.007	1.00	23.47



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TABLE 4

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

1320	O	GLY	A	988	0.225	11.626	18.802	1.00	23.29
1321	N	GLN	A	989	-0.674	12.988	17.272	1.00	23.22
1322	CA	GLN	A	989	-1.981	12.357	17.382	1.00	23.2
1323	C	GLN	A	989	-2.015	11.078	16.547	1.00	22.58
1324	O	GLN	A	989	-2.588	10.063	16.958	1.00	21.85
1325	CB	GLN	A	989	-3.089	13.295	16.893	1.00	24.05
1326	CG	GLN	A	989	-4.496	12.735	17.119	1.00	25.28
1327	CD	GLN	A	989	-5.571	13.479	16.339	1.00	26.65
1328	OE1	GLN	A	989	-6.75	13.486	16.727	1.00	27.07
1329	NE2	GLN	A	989	-5.176	14.097	15.225	1.00	26.95
1330	N	GLU	A	990	-1.394	11.139	15.375	1.00	22.13
1331	CA	GLU	A	990	-1.368	9.996	14.474	1.00	22.31
1332	C	GLU	A	990	-0.164	10.001	13.542	1.00	22.2
1333	O	GLU	A	990	0.282	11.054	13.073	1.00	22.06
1334	CB	GLU	A	990	-2.657	9.96	13.648	1.00	22.17
1335	CG	GLU	A	990	-2.725	8.823	12.647	1.00	23.33
1336	CD	GLU	A	990	-4.073	8.743	11.948	1.00	23.83
1337	OE1	GLU	A	990	-4.572	9.794	11.503	1.00	24.68
1338	OE2	GLU	A	990	-4.633	7.634	11.838	1.00	24.22
1339	N	VAL	A	991	0.357	8.813	13.27	1.00	21.96
1340	CA	VAL	A	991	1.501	8.688	12.395	1.00	22.14
1341	C	VAL	A	991	1.263	7.659	11.296	1.00	22.52
1342	O	VAL	A	991	0.742	6.57	11.539	1.00	22.12
1343	CB	VAL	A	991	2.778	8.311	13.2	1.00	22.19
1344	CG1	VAL	A	991	2.555	7.013	13.97	1.00	21.95
1345	CG2	VAL	A	991	3.971	8.183	12.261	1.00	21.97
1346	N	TYR	A	992	1.624	8.039	10.077	1.00	23.09
1347	CA	TYR	A	992	1.502	7.169	8.921	1.00	24.11
1348	C	TYR	A	992	2.91	6.641	8.656	1.00	25.01
1349	O	TYR	A	992	3.828	7.423	8.423	1.00	25.16
1350	CB	TYR	A	992	1.016	7.961	7.702	1.00	23.96
1351	CG	TYR	A	992	1.058	7.178	6.406	1.00	23.85
1352	CD1	TYR	A	992	0.126	6.171	6.144	1.00	23.47
1353	CD2	TYR	A	992	2.05	7.426	5.451	1.00	23.67
1354	CE1	TYR	A	992	0.181	5.43	4.963	1.00	23.87
1355	CE2	TYR	A	992	2.114	6.691	4.266	1.00	23.57
1356	CZ	TYR	A	992	1.178	5.696	4.028	1.00	23.9
1357	OH	TYR	A	992	1.231	4.969	2.861	1.00	24.12
1358	N	VAL	A	993	3.087	5.326	8.714	1.00	25.86
1359	CA	VAL	A	993	4.398	4.732	8.471	1.00	27.21

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TABLE 4

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

1360	C	VAL	A	993	4.253	3.609	7.463	1.00	28.3
1361	O	VAL	A	993	3.74	2.535	7.781	1.00	28.25
1362	CB	VAL	A	993	5.022	4.135	9.753	1.00	27
1363	CG1	VAL	A	993	6.473	3.72	9.477	1.00	26.79
1364	CG2	VAL	A	993	4.954	5.137	10.885	1.00	27.01
1365	N	LYS	A	994	4.707	3.866	6.245	1.00	29.82
1366	CA	LYS	A	994	4.625	2.883	5.177	1.00	31.48
1367	C	LYS	A	994	5.541	1.702	5.494	1.00	32.36
1368	O	LYS	A	994	6.631	1.877	6.051	1.00	32.56
1369	CB	LYS	A	994	5.035	3.537	3.856	1.00	31.91
1370	CG	LYS	A	994	4.348	2.965	2.634	1.00	32.65
1371	CD	LYS	A	994	4.683	3.776	1.393	1.00	32.92
1372	CE	LYS	A	994	3.939	3.245	0.182	1.00	33.24
1373	NZ	LYS	A	994	4.266	4.021	-1.047	1.00	34.01
1374	N	ALA	A	995	5.086	0.498	5.158	1.00	33.33
1375	CA	ALA	A	995	5.868	-0.714	5.396	1.00	34.15
1376	CB	ALA	A	995	5.085	-1.946	4.928	1.00	34.34
1377	C	ALA	A	995	7.195	-0.63	4.648	1.00	34.55
1378	OT1	ALA	A	995	8.253	-0.579	5.314	1.00	34.78
1379	OT2	ALA	A	995	7.153	-0.609	3.396	1.00	35.04
1380	N	ALA	A	999	7.343	-8.334	7.04	1.00	28.63
1381	CA	ALA	A	999	8.253	-7.474	7.851	1.00	28.39
1382	C	ALA	A	999	7.467	-6.718	8.925	1.00	27.87
1383	O	ALA	A	999	8.039	-6.227	9.897	1.00	28.22
1384	CB	ALA	A	999	8.987	-6.484	6.936	1.00	28.64
1385	N	LEU	A	0	6.154	-6.628	8.747	1.00	26.86
1386	CA	LEU	A	0	5.306	-5.93	9.706	1.00	25.72
1387	C	LEU	A	0	4.882	-6.869	10.831	1.00	24.5
1388	O	LEU	A	0	4.671	-8.06	10.605	1.00	24.53
1389	CB	LEU	A	0	4.052	-5.404	9.013	1.00	26.07
1390	CG	LEU	A	0	4.228	-4.631	7.71	1.00	26.55
1391	CD1	LEU	A	0	2.867	-4.465	7.03	1.00	26.64
1392	CD2	LEU	A	0	4.874	-3.28	7.998	1.00	27.08
1393	N	PRO	A	1	4.766	-6.345	12.063	1.00	23.43
1394	CA	PRO	A	1	4.353	-7.157	13.213	1.00	22.33
1395	C	PRO	A	1	2.831	-7.309	13.149	1.00	21.36
1396	O	PRO	A	1	2.103	-6.89	14.046	1.00	21.13
1397	CB	PRO	A	1	4.812	-6.319	14.399	1.00	22.44
1398	CG	PRO	A	1	4.6	-4.923	13.9	1.00	22.8
1399	CD	PRO	A	1	5.15	-4.986	12.492	1.00	23.03

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TABLE 4

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

1400	N	VAL	A	2	2.375	-7.906	12.056	1.00	20.41
1401	CA	VAL	A	2	0.963	-8.124	11.768	1.00	19.65
1402	C	VAL	A	2	0.102	-8.698	12.893	1.00	19.03
1403	O	VAL	A	2	-1.05	-8.302	13.059	1.00	18.7
1404	CB	VAL	A	2	0.824	-9.018	10.503	1.00	20.06
1405	CG1	VAL	A	2	-0.6	-9.525	10.362	1.00	20.62
1406	CG2	VAL	A	2	1.218	-8.211	9.258	1.00	19.87
1407	N	ARG	A	3	0.655	-9.626	13.664	1.00	18.49
1408	CA	ARG	A	3	-0.091	-10.251	14.746	1.00	18.31
1409	C	ARG	A	3	-0.443	-9.329	15.922	1.00	17.42
1410	O	ARG	A	3	-1.32	-9.645	16.722	1.00	16.99
1411	CB	ARG	A	3	0.677	-11.485	15.229	1.00	19.46
1412	CG	ARG	A	3	0.685	-12.602	14.187	1.00	21.34
1413	CD	ARG	A	3	1.964	-13.422	14.225	1.00	23.05
1414	NE	ARG	A	3	1.71	-14.804	14.609	1.00	25
1415	CZ	ARG	A	3	0.929	-15.647	13.936	1.00	25.62
1416	NH1	ARG	A	3	0.318	-15.256	12.824	1.00	26.18
1417	NH2	ARG	A	3	0.744	-16.879	14.39	1.00	25.58
1418	N	TRP	A	4	0.226	-8.185	16.013	1.00	16.54
1419	CA	TRP	A	4	-0.031	-7.23	17.089	1.00	16.35
1420	C	TRP	A	4	-0.731	-5.964	16.59	1.00	16.2
1421	O	TRP	A	4	-1.111	-5.105	17.383	1.00	15.9
1422	CB	TRP	A	4	1.291	-6.831	17.757	1.00	15.8
1423	CG	TRP	A	4	1.853	-7.863	18.692	1.00	15.76
1424	CD1	TRP	A	4	1.761	-7.872	20.059	1.00	15.82
1425	CD2	TRP	A	4	2.593	-9.039	18.334	1.00	15.58
1426	NE1	TRP	A	4	2.401	-8.979	20.572	1.00	15.51
1427	CE2	TRP	A	4	2.92	-9.711	19.537	1.00	15.57
1428	CE3	TRP	A	4	3.011	-9.591	17.114	1.00	15.57
1429	CZ2	TRP	A	4	3.648	-10.905	19.554	1.00	15.45
1430	CZ3	TRP	A	4	3.738	-10.785	17.133	1.00	15.51
1431	CH2	TRP	A	4	4.047	-11.425	18.346	1.00	15.43
1432	N	MET	A	5	-0.906	-5.855	15.277	1.00	16.15
1433	CA	MET	A	5	-1.504	-4.661	14.687	1.00	15.94
1434	C	MET	A	5	-3.027	-4.537	14.68	1.00	15.71
1435	O	MET	A	5	-3.747	-5.477	14.349	1.00	15.47
1436	CB	MET	A	5	-0.976	-4.487	13.261	1.00	15.87
1437	CG	MET	A	5	0.489	-4.097	13.195	1.00	15.9
1438	SD	MET	A	5	1.201	-4.254	11.541	1.00	16.6
1439	CE	MET	A	5	0.218	-3.063	10.625	1.00	15.15

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TABLE 4

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

1440	N	ALA	A	6	-3.503	-3.351	15.042	1.00	15.51
1441	CA	ALA	A	6	-4.932	-3.061	15.051	1.00	15.81
1442	C	ALA	A	6	-5.43	-3.078	13.6	1.00	16.14
1443	O	ALA	A	6	-4.649	-2.883	12.663	1.00	15.85
1444	CB	ALA	A	6	-5.179	-1.688	15.669	1.00	15.72
1445	N	ILE	A	7	-6.726	-3.315	13.418	1.00	16.3
1446	CA	ILE	A	7	-7.31	-3.354	12.079	1.00	16.6
1447	C	ILE	A	7	-6.954	-2.126	11.229	1.00	16.39
1448	O	ILE	A	7	-6.539	-2.263	10.076	1.00	16.41
1449	CB	ILE	A	7	-8.857	-3.463	12.151	1.00	17.23
1450	CG1	ILE	A	7	-9.263	-4.84	12.678	1.00	17.41
1451	CG2	ILE	A	7	-9.473	-3.224	10.771	1.00	17.38
1452	CD1	ILE	A	7	-10.736	-4.944	12.978	1.00	18.07
1453	N	GLU	A	8	-7.115	-0.932	11.796	1.00	15.91
1454	CA	GLU	A	8	-6.828	0.285	11.054	1.00	15.72
1455	C	GLU	A	8	-5.369	0.359	10.598	1.00	15.99
1456	O	GLU	A	8	-5.086	0.88	9.517	1.00	16.18
1457	CB	GLU	A	8	-7.191	1.529	11.879	1.00	15.3
1458	CG	GLU	A	8	-6.335	1.726	13.117	1.00	14.41
1459	CD	GLU	A	8	-6.979	1.182	14.374	1.00	14.12
1460	OE1	GLU	A	8	-7.785	0.229	14.277	1.00	13.53
1461	OE2	GLU'	A	8	-6.666	1.71	15.462	1.00	13.81
1462	N	SER	A	9	-4.448	-0.16	11.406	1.00	15.89
1463	CA	SER	A	9	-3.031	-0.141	11.043	1.00	16.09
1464	C	SER	A	9	-2.78	-1.102	9.881	1.00	16.35
1465	O	SER	A	9	-1.981	-0.82	8.985	1.00	15.94
1466	CB	SER	A	9	-2.158	-0.539	12.241	1.00	16.26
1467	OG	SER	A	9	-2.333	0.365	13.322	1.00	16.04
1468	N	LEU	A	10	-3.47	-2.239	9.908	1.00	16.43
1469	CA	LEU	A	10	-3.345	-3.236	8.851	1.00	16.74
1470	C	LEU	A	10	-3.879	-2.66	7.537	1.00	17.22
1471	O	LEU	A	10	-3.274	-2.83	6.473	1.00	17.12
1472	CB	LEU	A	10	-4.155	-4.488	9.201	1.00	16.24
1473	CG	LEU	A	10	-3.663	-5.337	10.375	1.00	16.54
1474	CD1	LEU	A	10	-4.675	-6.442	10.664	1.00	15.84
1475	CD2	LEU	A	10	-2.287	-5.917	10.049	1.00	16.06
1476	N	ASN	A	11	-5.014	-1.972	7.624	1.00	17.14
1477	CA	ASN	A	11	-5.642	-1.403	6.445	1.00	17.6
1478	C	ASN	A	11	-5.036	-0.121	5.912	1.00	17.56
1479	O	ASN	A	11	-4.953	0.05	4.698	1.00	18.05

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TABLE 4  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

1480	CB	ASN	A	11	-7.134	-1.147	6.696	1.00	18.02
1481	CG	ASN	A	11	-7.936	-2.425	6.805	1.00	18.35
1482	OD1	ASN	A	11	-7.531	-3.463	6.293	1.00	18.56
1483	ND2	ASN	A	11	-9.091	-2.35	7.457	1.00	19.02
1484	N	TYR	A	12	-4.6	0.768	6.803	1.00	17.45
1485	CA	TYR	A	12	-4.082	2.07	6.383	1.00	17.32
1486	C	TYR	A	12	-2.672	2.482	6.78	1.00	17.19
1487	O	TYR	A	12	-2.23	3.571	6.426	1.00	16.64
1488	CB	TYR	A	12	-5.054	3.15	6.86	1.00	18
1489	CG	TYR	A	12	-6.475	2.898	6.423	1.00	18.67
1490	CD1	TYR	A	12	-7.498	2.755	7.36	1.00	19.15
1491	CD2	TYR	A	12	-6.799	2.801	5.068	1.00	19.26
1492	CE1	TYR	A	12	-8.816	2.527	6.96	1.00	19.59
1493	CE2	TYR	A	12	-8.114	2.571	4.656	1.00	20.1
1494	CZ	TYR	A	12	-9.115	2.439	5.609	1.00	20.18
1495	OH	TYR	A	12	-10.416	2.239	5.203	1.00	21.53
1496	N	SER	A	13	-1.972	1.634	7.521	1.00	17.02
1497	CA	SER	A	13	-0.613	1.947	7.945	1.00	16.97
1498	C	SER	A	13	-0.558	3.157	8.865	1.00	16.54
1499	O	SER	A	13	0.43	3.085	8.89	1.00	16.16
1500	CB	SER	A	13	0.278	2.188	6.727	1.00	17.44
1501	OG	SER	A	13	0.254	1.058	5.871	1.00	18.39
1502	N	VAL	A	14	-1.627	3.378	9.617	1.00	16.38
1503	CA	VAL	A	14	-1.657	4.495	10.549	1.00	16.11
1504	C	VAL	A	14	-1.584	3.959	11.975	1.00	16.4
1505	O	VAL	A	14	-2.098	2.871	12.274	1.00	16.09
1506	CB	VAL	A	14	-2.936	5.362	10.374	1.00	16.28
1507	CG1	VAL	A	14	-2.894	6.08	9.029	1.00	15.46
1508	CG2	VAL	A	14	-4.188	4.494	10.479	1.00	16.02
1509	N	TYR	A	15	-0.925	4.722	12.847	1.00	16.39
1510	CA	TYR	A	15	-0.762	4.343	14.244	1.00	16
1511	C	TYR	A	15	-1.15	5.501	15.149	1.00	15.89
1512	O	TYR	A	15	-0.896	6.658	14.824	1.00	15.9
1513	CB	TYR	A	15	0.692	3.947	14.518	1.00	16.32
1514	CG	TYR	A	15	1.187	2.824	13.644	1.00	16.79
1515	CD1	TYR	A	15	1.588	3.064	12.33	1.00	17.37
1516	CD2	TYR	A	15	1.212	1.509	14.114	1.00	16.85
1517	CE1	TYR	A	15	2	2.019	11.498	1.00	17.91
1518	CE2	TYR	A	15	1.619	0.46	13.297	1.00	17.34
1519	CZ	TYR	A	15	2.009	0.721	11.989	1.00	17.99

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TABLE 4

STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

1520	OH	TYR	A	15	2.381	-0.316	11.163	1.00	18.67
1521	N	THR	A	16	-1.77	5.181	16.279	1.00	15.45
1522	CA	THR	A	16	-2.2	6.185	17.251	1.00	15.35
1523	C	THR	A	16	-2.12	5.548	18.635	1.00	15.17
1524	O	THR	A	16	-1.638	4.416	18.778	1.00	14.37
1525	CB	THR	A	16	-3.668	6.604	17.019	1.00	15.67
1526	OG1	THR	A	16	-4.527	5.481	17.281	1.00	15.84
1527	CG2	THR	A	16	-3.874	7.068	15.587	1.00	15.54
1528	N	THR	A	17	-2.596	6.268	19.649	1.00	14.94
1529	CA	THR	A	17	-2.587	5.727	21.002	1.00	15.18
1530	C	THR	A	17	-3.644	4.626	21.051	1.00	14.79
1531	O	THR	A	17	-3.529	3.658	21.805	1.00	14.31
1532	CB	THR	A	17	-2.908	6.812	22.065	1.00	15.51
1533	OG1	THR	A	17	-2.892	6.217	23.367	1.00	15.88
1534	CG2	THR	A	17	-4.287	7.413	21.831	1.00	15.94
1535	N	ASN	A	18	-4.669	4.767	20.218	1.00	14.55
1536	CA	ASN	A	18	-5.718	3.766	20.181	1.00	14.62
1537	C	ASN	A	18	-5.214	2.453	19.576	1.00	13.91
1538	O	ASN	A	18	-5.607	1.38	20.023	1.00	13.76
1539	CB	ASN	A	18	-6.942	4.294	19.428	1.00	15.58
1540	CG	ASN	A	18	-7.665	5.397	20.202	1.00	17.09
1541	OD1	ASN	A	18	-7.896	5.277	21.409	1.00	17.53
1542	ND2	ASN	A	18	-8.03	6.471	19.508	1.00	17.64
1543	N	SER	A	19	-4.343	2.52	18.574	1.00	13.48
1544	CA	SER	A	19	-3.825	1.281	18.012	1.00	12.99
1545	C	SER	A	19	-2.804	0.69	18.994	1.00	12.72
1546	O	SER	A	19	-2.618	-0.519	19.042	1.00	12.64
1547	CB	SER	A	19	-3.207	1.5	16.623	1.00	12.89
1548	OG	SER	A	19	-2.16	2.446	16.629	1.00	13.04
1549	N	ASP	A	20	-2.153	1.54	19.787	1.00	12.55
1550	CA	ASP	A	20	-1.206	1.038	20.784	1.00	12.12
1551	C	ASP	A	20	-1.988	0.185	21.782	1.00	12
1552	O	ASP	A	20	-1.52	-0.862	22.229	1.00	12.02
1553	CB	ASP	A	20	-0.521	2.182	21.544	1.00	11.79
1554	CG	ASP	A	20	0.701	2.725	20.825	1.00	11.43
1555	OD1	ASP	A	20	1.212	2.068	19.896	1.00	11.59
1556	OD2	ASP	A	20	1.167	3.816	21.202	1.00	12.11
1557	N	VAL	A	21	-3.181	0.65	22.131	1.00	11.85
1558	CA	VAL	A	21	-4.044	-0.063	23.061	1.00	11.81
1559	C	VAL	A	21	-4.406	-1.445	22.512	1.00	12.05

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TABLE 4

STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

1560	O	VAL	A	21	-4.468	-2.413	23.266	1.00	11.83
1561	CB	VAL	A	21	-5.328	0.752	23.351	1.00	11.82
1562	CG1	VAL	A	21	-6.397	-0.136	23.992	1.00	11.72
1563	CG2	VAL	A	21	-4.993	1.909	24.278	1.00	11.48
1564	N	TRP	A	22	-4.641	-1.538	21.201	1.00	11.91
1565	CA	TRP	A	22	-4.963	-2.827	20.589	1.00	11.9
1566	C	TRP	A	22	-3.764	-3.739	20.801	1.00	11.79
1567	O	TRP	A	22	-3.905	-4.88	21.245	1.00	11.98
1568	CB	TRP	A	22	-5.243	-2.666	19.084	1.00	11.73
1569	CG	TRP	A	22	-5.492	-3.971	18.35	1.00	11.66
1570	CD1	TRP	A	22	-4.601	-5.005	18.168	1.00	11.66
1571	CD2	TRP	A	22	-6.701	-4.368	17.686	1.00	11.35
1572	NE1	TRP	A	22	-5.184	-6.011	17.437	1.00	11.5
1573	CE2	TRP	A	22	-6.471	-5.647	17.127	1.00	11.5
1574	CE3	TRP	A	22	-7.956	-3.766	17.508	1.00	11.36
1575	CZ2	TRP	A	22	-7.454	-6.337	16.399	1.00	11.52
1576	CZ3	TRP	A	22	-8.935	-4.453	16.784	1.00	11.19
1577	CH2	TRP	A	22	-8.675	-5.725	16.241	1.00	11.31
1578	N	SER	A	23	-2.576	-3.231	20.487	1.00	11.79
1579	CA	SER	A	23	-1.363	-4.015	20.663	1.00	11.42
1580	C	SER	A	23	-1.166	-4.356	22.138	1.00	11.51
1581	O	SER	A	23	-0.613	-5.406	22.476	1.00	11.43
1582	CB	SER	A	23	-0.158	-3.247	20.125	1.00	11.51
1583	OG	SER	A	23	-0.307	-3.016	18.736	1.00	10.99
1584	N	TYR	A	24	-1.622	-3.474	23.024	1.00	11.54
1585	CA	TYR	A	24	-1.494	-3.752	24.448	1.00	11.52
1586	C	TYR	A	24	-2.348	-4.978	24.769	1.00	11.46
1587	O	TYR	A	24	-1.932	-5.86	25.521	1.00	11.54
1588	CB	TYR	A	24	-1.963	-2.574	25.299	1.00	11.3
1589	CG	TYR	A	24	-1.909	-2.906	26.771	1.00	11.36
1590	CD1	TYR	A	24	-0.726	-2.758	27.501	1.00	11.15
1591	CD2	TYR	A	24	-3.015	-3.449	27.415	1.00	11.46
1592	CE1	TYR	A	24	-0.654	-3.15	28.843	1.00	11.7
1593	CE2	TYR	A	24	-2.956	-3.848	28.747	1.00	11.8
1594	CZ	TYR	A	24	-1.777	-3.696	29.454	1.00	11.79
1595	OH	TYR	A	24	-1.736	-4.087	30.768	1.00	12.41
1596	N	GLY	A	25	-3.549	-5.023	24.198	1.00	11.5
1597	CA	GLY	A	25	-4.426	-6.162	24.417	1.00	11.16
1598	C	GLY	A	25	-3.749	-7.469	24.024	1.00	11.11
1599	O	GLY	A	25	-3.883	-8.478	24.716	1.00	11.06

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TABLE 4

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

1600	N	VAL	A	26	-3.03	-7.461	22.905	1.00	10.99
1601	CA	VAL	A	26	-2.33	-8.66	22.461	1.00	11.29
1602	C	VAL	A	26	-1.204	-9.002	23.448	1.00	11.2
1603	O	VAL	A	26	-0.967	-10.172	23.76	1.00	11.64
1604	CB	VAL	A	26	-1.728	-8.476	21.061	1.00	11.27
1605	CG1	VAL	A	26	-1.111	-9.789	20.601	1.00	11.65
1606	CG2	VAL	A	26	-2.813	-8.021	20.079	1.00	11.41
1607	N	LEU	A	27	-0.508	-7.975	23.926	1.00	11.04
1608	CA	LEU	A	27	0.563	-8.157	24.899	1.00	11.12
1609	C	LEU	A	27	-0.003	-8.851	26.141	1.00	10.94
1610	O	LEU	A	27	0.62	-9.758	26.691	1.00	10.54
1611	CB	LEU	A	27	1.151	-6.799	25.301	1.00	11.51
1612	CG	LEU	A	27	1.965	-6.813	26.603	1.00	12.21
1613	CD1	LEU	A	27	3.172	-7.712	26.406	1.00	12.29
1614	CD2	LEU	A	27	2.405	-5.407	26.984	1.00	12.9
1615	N	LEU	A	28	-1.181	-8.406	26.578	1.00	10.71
1616	CA	LEU	A	28	-1.852	-8.98	27.751	1.00	10.96
1617	C	LEU	A	28	-2.122	-10.463	27.506	1.00	10.92
1618	O	LEU	A	28	-2.011	-11.295	28.409	1.00	10.68
1619	CB	LEU	A	28	-3.174	-8.248	28.013	1.00	11.03
1620	CG	LEU	A	28	-4.048	-8.676	29.199	1.00	11.52
1621	CD1	LEU	A	28	-3.216	-8.775	30.483	1.00	11.51
1622	CD2	LEU	A	28	-5.173	-7.647	29.371	1.00	11.54
1623	N	TRP	A	29	-2.474	-10.784	26.267	1.00	10.93
1624	CA	TRP	A	29	-2.74	-12.159	25.887	1.00	11.22
1625	C	TRP	A	29	-1.411	-12.934	25.974	1.00	11.18
1626	O	TRP	A	29	-1.376	-14.065	26.456	1.00	11.11
1627	CB	TRP	A	29	-3.296	-12.197	24.461	1.00	11.46
1628	CG	TRP	A	29	-3.762	-13.554	24.009	1.00	12.16
1629	CD1	TRP	A	29	-5.028	-14.052	24.092	1.00	11.81
1630	CD2	TRP	A	29	-2.975	-14.562	23.364	1.00	12.22
1631	NE1	TRP	A	29	-5.082	-15.303	23.531	1.00	12.18
1632	CE2	TRP	A	29	-3.835	-15.642	23.076	1.00	12.68
1633	CE3	TRP	A	29	-1.625	-14.656	22.999	1.00	12.69
1634	CZ2	TRP	A	29	-3.391	-16.812	22.435	1.00	13.04
1635	CZ3	TRP	A	29	-1.18	-15.817	22.36	1.00	12.84
1636	CH2	TRP	A	29	-2.064	-16.878	22.086	1.00	13.47
1637	N	GLU	A	30	-0.324	-12.325	25.505	1.00	10.88
1638	CA	GLU	A	30	0.986	-12.975	25.571	1.00	11.55
1639	C	GLU	A	30	1.338	-13.3	27.028	1.00	11.83



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TABLE 4

STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

1640	O	GLU	A	30	1.771	-14.412	27.344	1.00	11.9
1641	CB	GLU	A	30	2.083	-12.068	25.002	1.00	11.12
1642	CG	GLU	A	30	2	-11.803	23.512	1.00	11.19
1643	CD	GLU	A	30	3.181	-10.988	23.019	1.00	11.23
1644	OE1	GLU	A	30	4.214	-11.595	22.66	1.00	11.39
1645	OE2	GLU	A	30	3.08	-9.743	23.006	1.00	10.91
1646	N	ILE	A	31	1.148	-12.317	27.906	1.00	11.87
1647	CA	ILE	A	31	1.446	-12.481	29.324	1.00	12.17
1648	C	ILE	A	31	0.673	-13.641	29.925	1.00	12.56
1649	O	ILE	A	31	1.258	-14.555	30.513	1.00	13.11
1650	CB	ILE	A	31	1.103	-11.198	30.122	1.00	11.8
1651	CG1	ILE	A	31	2.097	-10.088	29.769	1.00	11.82
1652	CG2	ILE	A	31	1.123	-11.49	31.62	1.00	11.74
1653	CD1	ILE	A	31	1.769	-8.748	30.389	1.00	11.42
1654	N	VAL	A	32	-0.644	-13.596	29.765	1.00	12.73
1655	CA	VAL	A	32	-1.54	-14.611	30.304	1.00	12.87
1656	C	VAL	A	32	-1.255	-16.01	29.77	1.00	13.22
1657	O	VAL	A	32	-1.368	-16.99	30.504	1.00	13.01
1658	CB	VAL	A	32	-3.011	-14.239	30.009	1.00	12.87
1659	CG1	VAL	A	32	-3.939	-15.408	30.338	1.00	12.95
1660	CG2	VAL	A	32	-3.394	-13.003	30.812	1.00	12.98
1661	N	SER	A	33	-0.893	-16.095	28.493	1.00	13.47
1662	CA	SER	A	33	-0.603	-17.374	27.861	1.00	13.64
1663	C	SER	A	33	0.854	-17.773	28.042	1.00	13.85
1664	O	SER	A	33	1.34	-18.681	27.369	1.00	13.47
1665	CB	SER	A	33	-0.928	-17.316	26.366	1.00	14.04
1666	OG	SER	A	33	0.009	-16.511	25.664	1.00	14.78
1667	N	LEU	A	34	1.544	-17.082	28.946	1.00	14.07
1668	CA	LEU	A	34	2.943	-17.355	29.234	1.00	14.55
1669	C	LEU	A	34	3.826	-17.292	27.988	1.00	15.14
1670	O	LEU	A	34	4.737	-18.111	27.805	1.00	15.3
1671	CB	LEU	A	34	3.079	-18.724	29.918	1.00	14.65
1672	CG	LEU	A	34	2.272	-18.844	31.218	1.00	14.77
1673	CD1	LEU	A	34	2.362	-20.263	31.766	1.00	15.47
1674	CD2	LEU	A	34	2.793	-17.838	32.241	1.00	14.77
1675	N	GLY	A	35	3.551	-16.317	27.129	1.00	15.14
1676	CA	GLY	A	35	4.352	-16.152	25.929	1.00	15.56
1677	C	GLY	A	35	3.905	-16.843	24.654	1.00	15.83
1678	O	GLY	A	35	4.724	-17.088	23.768	1.00	16.25
1679	N	GLY	A	36	2.62	-17.154	24.533	1.00	15.91

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TABLE 4  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

1680	CA	GLY	A	36	2.166	-17.806	23.323	1.00	15.69
1681	C	GLY	A	36	2.244	-16.859	22.137	1.00	16.26
1682	O	GLY	A	36	2.222	-15.635	22.302	1.00	16.09
1683	N	THR	A	37	2.358	-17.417	20.937	1.00	16.25
1684	CA	THR	A	37	2.406	-16.606	19.737	1.00	16.53
1685	C	THR	A	37	0.944	-16.381	19.333	1.00	17.15
1686	O	THR	A	37	0.173	-17.329	19.196	1.00	16.91
1687	CB	THR	A	37	3.192	-17.329	18.602	1.00	16.63
1688	OG1	THR	A	37	4.537	-17.577	19.036	1.00	16.32
1689	CG2	THR	A	37	3.238	-16.477	17.341	1.00	16
1690	N	PRO	A	38	0.539	-15.112	19.169	1.00	17.69
1691	CA	PRO	A	38	-0.843	-14.787	18.786	1.00	18.01
1692	C	PRO	A	38	-1.284	-15.417	17.463	1.00	18.54
1693	O	PRO	A	38	-0.549	-15.395	16.478	1.00	17.95
1694	CB	PRO	A	38	-0.835	-13.258	18.707	1.00	17.82
1695	CG	PRO	A	38	0.298	-12.855	19.636	1.00	17.75
1696	CD	PRO	A	38	1.348	-13.889	19.332	1.00	17.8
1697	N	TYR	A	39	-2.49	-15.977	17.457	1.00	19.67
1698	CA	TYR	A	39	-3.067	-16.586	16.261	1.00	21.25
1699	C	TYR	A	39	-2.271	-17.782	15.73	1.00	22.78
1700	O	TYR	A	39	-2.387	-18.148	14.559	1.00	22.71
1701	CB	TYR	A	39	-3.196	-15.527	15.162	1.00	20.51
1702	CG	TYR	A	39	-3.838	-14.234	15.628	1.00	20.02
1703	CD1	TYR	A	39	-5.195	-14.177	15.942	1.00	19.76
1704	CD2	TYR	A	39	-3.087	-13.066	15.745	1.00	19.58
1705	CE1	TYR	A	39	-5.791	-12.983	16.357	1.00	19.63
1706	CE2	TYR	A	39	-3.669	-11.872	16.162	1.00	19.6
1707	CZ	TYR	A	39	-5.019	-11.835	16.465	1.00	19.36
1708	OH	TYR	A	39	-5.592	-10.653	16.875	1.00	19.18
1709	N	CYS	A	40	-1.468	-18.388	16.594	1.00	24.58
1710	CA	CYS	A	40	-0.665	-19.545	16.218	1.00	26.99
1711	C	CYS	A	40	-1.527	-20.641	15.585	1.00	27.93
1712	O	CYS	A	40	-2.58	-20.996	16.114	1.00	27.79
1713	CB	CYS	A	40	0.02	-20.099	17.459	1.00	27.98
1714	SG	CYS	A	40	1.296	-21.367	17.193	1.00	29.19
1715	N	GLY	A	41	-1.07	-21.181	14.46	1.00	29.27
1716	CA	GLY	A	41	-1.821	-22.231	13.791	1.00	31.23
1717	C	GLY	A	41	-2.829	-21.635	12.835	1.00	32.69
1718	O	GLY	A	41	-3.743	-22.311	12.36	1.00	32.92
1719	N	MET	A	42	-2.651	-20.35	12.557	1.00	34.11

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TABLE 4

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

1720	CA	MET	A	42	-3.528	-19.613	11.659	1.00	35.56
1721	C	MET	A	42	-2.633	-18.799	10.729	1.00	36.24
1722	O	MET	A	42	-1.672	-18.171	11.176	1.00	36.36
1723	CB	MET	A	42	-4.428	-18.683	12.484	1.00	36.15
1724	CG	MET	A	42	-5.565	-18.019	11.736	1.00	36.59
1725	SD	MET	A	42	-6.454	-16.855	12.818	1.00	37.72
1726	CE	MET	A	42	-7.448	-17.96	13.781	1.00	37.06
1727	N	THR	A	43	-2.933	-18.824	9.435	1.00	37.12
1728	CA	THR	A	43	-2.148	-18.065	8.468	1.00	37.98
1729	C	THR	A	43	-2.619	-16.614	8.473	1.00	38.6
1730	O	THR	A	43	-3.748	-16.324	8.875	1.00	38.7
1731	CB	THR	A	43	-2.308	-18.636	7.043	1.00	38.04
1732	OG1	THR	A	43	-3.688	-18.587	6.659	1.00	37.9
1733	CG2	THR	A	43	-1.826	-20.079	6.99	1.00	38.16
1734	N	CYS	A	44	-1.757	-15.704	8.03	1.00	39.45
1735	CA	CYS	A	44	-2.103	-14.287	7.987	1.00	40.41
1736	C	CYS	A	44	-3.36	-14.035	7.148	1.00	40.77
1737	O	CYS	A	44	-4.207	-13.215	7.507	1.00	40.74
1738	CB	CYS	A	44	-0.932	-13.477	7.424	1.00	40.54
1739	SG	CYS	A	44	0.547	-13.485	8.468	1.00	41.63
1740	N	ALA	A	45	-3.474	-14.745	6.032	1.00	41.24
1741	CA	ALA	A	45	-4.625	-14.598	5.148	1.00	41.74
1742	C	ALA	A	45	-5.909	-14.856	5.924	1.00	41.99
1743	O	ALA	A	45	-6.896	-14.14	5.767	1.00	41.99
1744	CB	ALA	A	45	-4.513	-15.569	3.978	1.00	41.66
1745	N	GLU	A	46	-5.891	-15.889	6.761	1.00	42.39
1746	CA	GLU	A	46	-7.051	-16.225	7.574	1.00	42.85
1747	C	GLU	A	46	-7.295	-15.09	8.56	1.00	42.93
1748	O	GLU	A	46	-8.436	-14.784	8.904	1.00	42.94
1749	CB	GLU	A	46	-6.802	-17.521	8.344	1.00	43.29
1750	CG	GLU	A	46	-6.766	-18.768	7.482	1.00	44
1751	CD	GLU	A	46	-6.186	-19.958	8.218	1.00	44.34
1752	OE1	GLU	A	46	-4.969	-19.949	8.495	1.00	44.84
1753	OE2	GLU	A	46	-6.943	-20.9	8.529	1.00	44.7
1754	N	LEU	A	47	-6.204	-14.473	9.004	1.00	43.05
1755	CA	LEU	A	47	-6.255	-13.369	9.953	1.00	43.18
1756	C	LEU	A	47	-6.906	-12.153	9.3	1.00	43.2
1757	O	LEU	A	47	-7.916	-11.633	9.78	1.00	43.13
1758	CB	LEU	A	47	-4.836	-12.996	10.392	1.00	43.37
1759	CG	LEU	A	47	-4.514	-12.722	11.864	1.00	43.64

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## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

1760	CD1	LEU	A	47	-3.168	-12.013	11.933	1.00	43.63
1761	CD2	LEU	A	47	-5.588	-11.87	12.515	1.00	43.61
1762	N	TYR	A	48	-6.301	-11.708	8.203	1.00	43.21
1763	CA	TYR	A	48	-6.762	-10.549	7.445	1.00	43.14
1764	C	TYR	A	48	-8.212	-10.675	7.021	1.00	42.93
1765	O	TYR	A	48	-8.915	-9.68	6.864	1.00	43.02
1766	CB	TYR	A	48	-5.905	-10.386	6.195	1.00	43.25
1767	CG	TYR	A	48	-4.435	-10.222	6.478	1.00	43.71
1768	CD1	TYR	A	48	-3.485	-10.504	5.496	1.00	43.88
1769	CD2	TYR	A	48	-3.988	-9.753	7.713	1.00	43.8
1770	CE1	TYR	A	48	-2.127	-10.323	5.735	1.00	44.01
1771	CE2	TYR	A	48	-2.63	-9.566	7.961	1.00	43.96
1772	CZ	TYR	A	48	-1.706	-9.852	6.969	1.00	44.01
1773	OH	TYR	A	48	-0.362	-9.669	7.203	1.00	44.14
1774	N	GLU	A	49	-8.647	-11.914	6.836	1.00	42.72
1775	CA	GLU	A	49	-10.001	-12.21	6.398	1.00	42.33
1776	C	GLU	A	49	-10.969	-12.357	7.562	1.00	41.62
1777	O	GLU	A	49	-12.176	-12.161	7.407	1.00	41.65
1778	CB	GLU	A	49	-9.979	-13.505	5.588	1.00	43.19
1779	CG	GLU	A	49	-11.279	-13.873	4.909	1.00	44.25
1780	CD	GLU	A	49	-11.197	-15.238	4.247	1.00	44.94
1781	OE1	GLU	A	49	-11.197	-16.256	4.977	1.00	45.2
1782	OE2	GLU	A	49	-11.117	-15.293	2.998	1.00	45.34
1783	N	LYS	A	50	-10.438	-12.694	8.731	1.00	40.42
1784	CA	LYS	A	50	-11.278	-12.902	9.898	1.00	39.36
1785	C	LYS	A	50	-11.407	-11.698	10.833	1.00	38.27
1786	O	LYS	A	50	-12.471	-11.476	11.411	1.00	37.89
1787	CB	LYS	A	50	-10.773	-14.125	10.669	1.00	39.86
1788	CG	LYS	A	50	-11.853	-15.143	10.987	1.00	40.67
1789	CD	LYS	A	50	-11.263	-16.454	11.485	1.00	41.21
1790	CE	LYS	A	50	-12.349	-17.363	12.055	1.00	41.79
1791	NZ	LYS	A	50	-13.417	-17.689	11.064	1.00	42.4
1792	N	LEU	A	51	-10.336	-10.925	10.985	1.00	37.03
1793	CA	LEU	A	51	-10.382	-9.757	11.861	1.00	36.16
1794	C	LEU	A	51	-11.552	-8.833	11.541	1.00	35.78
1795	O	LEU	A	51	-12.281	-8.41	12.44	1.00	35.55
1796	CB	LEU	A	51	-9.07	-8.968	11.791	1.00	35.8
1797	CG	LEU	A	51	-7.912	-9.511	12.631	1.00	35.55
1798	CD1	LEU	A	51	-6.743	-8.553	12.564	1.00	35.29
1799	CD2	LEU	A	51	-8.362	-9.688	14.076	1.00	35.23

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TABLE 4

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

1800	N	PRO	A	52	-11.754	-8.509	10.253	1.00	35.36
1801	CA	PRO	A	52	-12.864	-7.624	9.889	1.00	35.14
1802	C	PRO	A	52	-14.23	-8.237	10.193	1.00	34.76
1803	O	PRO	A	52	-15.191	-7.519	10.455	1.00	34.99
1804	CB	PRO	A	52	-12.639	-7.386	8.397	1.00	35.25
1805	CG	PRO	A	52	-12.001	-8.664	7.954	1.00	35.59
1806	CD	PRO	A	52	-11.01	-8.936	9.056	1.00	35.35
1807	N	GLN	A	53	-14.309	-9.564	10.159	1.00	34.24
1808	CA	GLN	A	53	-15.558	-10.263	10.442	1.00	33.73
1809	C	GLN	A	53	-15.857	-10.257	11.944	1.00	32.97
1810	O	GLN	A	53	-16.925	-10.699	12.377	1.00	32.96
1811	CB	GLN	A	53	-15.481	-11.709	9.939	1.00	34.32
1812	CG	GLN	A	53	-15.204	-11.83	8.443	1.00	35.17
1813	CD	GLN	A	53	-15.065	-13.275	7.98	1.00	35.64
1814	OE1	GLN	A	53	-14.869	-13.542	6.793	1.00	35.85
1815	NE2	GLN	A	53	-15.165	-14.214	8.917	1.00	35.88
1816	N	GLY	A	54	-14.908	-9.78	12.732	1.00	31.98
1817	CA	GLY	A	54	-15.096	-9.705	14.171	1.00	30.51
1818	C	GLY	A	54	-14.317	-10.756	14.941	1.00	29.68
1819	O	GLY	A	54	-14.447	-10.864	16.162	1.00	29.69
1820	N	TYR	A	55	-13.508	-11.546	14.244	1.00	28.8
1821	CA	TYR	A	55	-12.727	-12.568	14.927	1.00	27.78
1822	C	TYR	A	55	-11.672	-11.925	15.815	1.00	26.58
1823	O	TYR	A	55	-11.065	-10.92	15.446	1.00	26.45
1824	CB	TYR	A	55	-12.038	-13.498	13.928	1.00	28.4
1825	CG	TYR	A	55	-11.246	-14.587	14.615	1.00	29.51
1826	CD1	TYR	A	55	-9.873	-14.453	14.833	1.00	29.72
1827	CD2	TYR	A	55	-11.886	-15.73	15.104	1.00	29.89
1828	CE1	TYR	A	55	-9.156	-15.432	15.525	1.00	30.22
1829	CE2	TYR	A	55	-11.184	-16.71	15.794	1.00	30.29
1830	CZ	TYR	A	55	-9.821	-16.558	16.001	1.00	30.46
1831	OH	TYR	A	55	-9.135	-17.54	16.676	1.00	30.61
1832	N	ARG	A	56	-11.463	-12.513	16.985	1.00	25.19
1833	CA	ARG	A	56	-10.48	-12.015	17.935	1.00	24.13
1834	C	ARG	A	56	-9.787	-13.186	18.606	1.00	23.63
1835	O	ARG	A	56	-10.259	-14.321	18.538	1.00	23.51
1836	CB	ARG	A	56	-11.164	-11.151	18.999	1.00	23.67
1837	CG	ARG	A	56	-11.761	-9.856	18.466	1.00	22.8
1838	CD	ARG	A	56	-10.675	-8.897	18.01	1.00	22.03
1839	NE	ARG	A	56	-11.215	-7.59	17.641	1.00	21.56

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

1840	CZ	ARG	A	56	-11.738	-7.292	16.456	1.00	21.6
1841	NH1	ARG	A	56	-11.8	-8.208	15.498	1.00	21.35
1842	NH2	ARG	A	56	-12.194	-6.069	16.225	1.00	21.25
1843	N	LEU	A	57	-8.655	-12.915	19.243	1.00	22.92
1844	CA	LEU	A	57	-7.933	-13.964	19.949	1.00	22.42
1845	C	LEU	A	57	-8.883	-14.611	20.952	1.00	22.38
1846	O	LEU	A	57	-9.695	-13.927	21.577	1.00	21.73
1847	CB	LEU	A	57	-6.719	-13.382	20.681	1.00	21.47
1848	CG	LEU	A	57	-5.52	-13.02	19.804	1.00	21.16
1849	CD1	LEU	A	57	-4.579	-12.095	20.565	1.00	20.47
1850	CD2	LEU	A	57	-4.814	-14.306	19.366	1.00	20.45
1851	N	GLU	A	58	-8.781	-15.928	21.092	1.00	22.66
1852	CA	GLU	A	58	-9.633	-16.665	22.014	1.00	23.34
1853	C	GLU	A	58	-9.134	-16.56	23.445	1.00	22.61
1854	O	GLU	A	58	-7.944	-16.353	23.686	1.00	22.47
1855	CB	GLU	A	58	-9.684	-18.141	21.63	1.00	24.65
1856	CG	GLU	A	58	-10.26	-18.411	20.265	1.00	27.25
1857	CD	GLU	A	58	-10.403	-19.894	20.014	1.00	28.83
1858	OE1	GLU	A	58	-11.183	-20.544	20.752	1.00	29.55
1859	OE2	GLU	A	58	-9.727	-20.407	19.093	1.00	29.86
1860	N	LYS	A	59	-10.052	-16.716	24.392	1.00	22.04
1861	CA	LYS	A	59	-9.694	-16.651	25.796	1.00	21.6
1862	C	LYS	A	59	-8.872	-17.867	26.179	1.00	21.16
1863	O	LYS	A	59	-9.306	-19	25.989	1.00	20.93
1864	CB	LYS	A	59	-10.941	-16.6	26.68	1.00	21.71
1865	CG	LYS	A	59	-10.626	-16.481	28.171	1.00	22.13
1866	CD	LYS	A	59	-11.889	-16.365	29.02	1.00	22.65
1867	CE	LYS	A	59	-12.567	-17.711	29.203	1.00	22.82
1868	NZ	LYS	A	59	-11.685	-18.631	29.982	1.00	23.26
1869	N	PRO	A	60	-7.65	-17.645	26.687	1.00	20.9
1870	CA	PRO	A	60	-6.807	-18.767	27.093	1.00	20.71
1871	C	PRO	A	60	-7.568	-19.501	28.194	1.00	20.6
1872	O	PRO	A	60	-8.249	-18.876	29.014	1.00	20.2
1873	CB	PRO	A	60	-5.548	-18.077	27.607	1.00	20.99
1874	CG	PRO	A	60	-5.461	-16.867	26.722	1.00	20.87
1875	CD	PRO	A	60	-6.893	-16.381	26.714	1.00	20.93
1876	N	LEU	A	61	-7.462	-20.822	28.203	1.00	20.44
1877	CA	LEU	A	61	-8.16	-21.635	29.19	1.00	20.47
1878	C	LEU	A	61	-7.801	-21.339	30.645	1.00	20.33
1879	O	LEU	A	61	-8.616	-21.549	31.543	1.00	20.44

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TABLE 4  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

1880	CB	LEU	A	61	-7.93	-23.114	28.882	1.00	20.74
1881	CG	LEU	A	61	-8.415	-23.51	27.486	1.00	20.95
1882	CD1	LEU	A	61	-8.049	-24.96	27.2	1.00	20.93
1883	CD2	LEU	A	61	-9.923	-23.295	27.389	1.00	20.84
1884	N	ASN	A	62	-6.589	-20.852	30.882	1.00	19.95
1885	CA	ASN	A	62	-6.155	-20.525	32.238	1.00	19.71
1886	C	ASN	A	62	-6.509	-19.073	32.605	1.00	19.74
1887	O	ASN	A	62	-6.12	-18.588	33.668	1.00	19.59
1888	CB	ASN	A	62	-4.64	-20.716	32.354	1.00	19.4
1889	CG	ASN	A	62	-3.861	-19.69	31.544	1.00	19.22
1890	OD1	ASN	A	62	-4.2	-19.403	30.399	1.00	19.24
1891	ND2	ASN	A	62	-2.808	-19.138	32.136	1.00	19.09
1892	N	CYS	A	63	-7.261	-18.398	31.737	1.00	19.8
1893	CA	CYS	A	63	-7.626	-16.992	31.95	1.00	20.21
1894	C	CYS	A	63	-9.056	-16.729	32.444	1.00	20.57
1895	O	CYS	A	63	-10.021	-17.259	31.904	1.00	20.48
1896	CB	CYS	A	63	-7.384	-16.207	30.653	1.00	19.64
1897	SG	CYS	A	63	-7.553	-14.413	30.768	1.00	19.5
1898	N	ASP	A	64	-9.169	-15.892	33.473	1.00	21.19
1899	CA	ASP	A	64	-10.458	-15.513	34.051	1.00	21.81
1900	C	ASP	A	64	-11.215	-14.614	33.062	1.00	21.77
1901	O	ASP	A	64	-10.602	-13.859	32.301	1.00	21.16
1902	CB	ASP	A	64	-10.233	-14.744	35.359	1.00	22.88
1903	CG	ASP	A	64	-11.535	-14.374	36.058	1.00	24.11
1904	OD1	ASP	A	64	-12.155	-15.263	36.683	1.00	25.06
1905	OD2	ASP	A	64	-11.946	-13.196	35.973	1.00	24.83
1906	N	ASP	A	65	-12.542	-14.704	33.077	1.00	21.59
1907	CA	ASP	A	65	-13.377	-13.898	32.198	1.00	21.78
1908	C	ASP	A	65	-13.071	-12.406	32.287	1.00	21.48
1909	O	ASP	A	65	-13.043	-11.713	31.268	1.00	21.38
1910	CB	ASP	A	65	-14.867	-14.09	32.52	1.00	22.54
1911	CG	ASP	A	65	-15.434	-15.386	31.969	1.00	23.52
1912	OD1	ASP	A	65	-14.928	-15.878	30.943	1.00	23.77
1913	OD2	ASP	A	65	-16.414	-15.903	32.555	1.00	24.8
1914	N	GLU	A	66	-12.849	-11.913	33.503	1.00	20.89
1915	CA	GLU	A	66	-12.592	-10.492	33.691	1.00	20.56
1916	C	GLU	A	66	-11.361	-9.993	32.946	1.00	19.61
1917	O	GLU	A	66	-11.388	-8.916	32.361	1.00	19.45
1918	CB	GLU	A	66	-12.474	-10.152	35.182	1.00	21.27
1919	CG	GLU	A	66	-12.604	-8.658	35.449	1.00	23

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TABLE 4  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

1920	CD	GLU	A	66	-12.731	-8.311	36.926	1.00	23.97
1921	OE1	GLU	A	66	-13.335	-9.105	37.682	1.00	24.44
1922	OE2	GLU	A	66	-12.243	-7.229	37.324	1.00	24.62
1923	N	VAL	A	67	-10.28	-10.764	32.97	1.00	18.88
1924	CA	VAL	A	67	-9.065	-10.357	32.27	1.00	17.66
1925	C	VAL	A	67	-9.326	-10.399	30.765	1.00	17.16
1926	O	VAL	A	67	-8.911	-9.507	30.023	1.00	17
1927	CB	VAL	A	67	-7.875	-11.286	32.612	1.00	17.58
1928	CG1	VAL	A	67	-6.639	-10.864	31.819	1.00	17.27
1929	CG2	VAL	A	67	-7.581	-11.229	34.113	1.00	17.22
1930	N	TYR	A	68	-10.029	-11.434	30.318	1.00	16.57
1931	CA	TYR	A	68	-10.341	-11.559	28.9	1.00	16.25
1932	C	TYR	A	68	-11.215	-10.39	28.436	1.00	16.09
1933	O	TYR	A	68	-10.997	-9.838	27.362	1.00	15.81
1934	CB	TYR	A	68	-11.056	-12.879	28.62	1.00	15.82
1935	CG	TYR	A	68	-11.282	-13.128	27.148	1.00	16.08
1936	CD1	TYR	A	68	-10.203	-13.206	26.262	1.00	15.63
1937	CD2	TYR	A	68	-12.573	-13.271	26.634	1.00	15.88
1938	CE1	TYR	A	68	-10.405	-13.422	24.903	1.00	15.91
1939	CE2	TYR	A	68	-12.786	-13.486	25.275	1.00	15.77
1940	CZ	TYR	A	68	-11.698	-13.56	24.419	1.00	15.97
1941	OH	TYR	A	68	-11.902	-13.772	23.082	1.00	15.9
1942	N	ASP	A	69	-12.202	-10.015	29.246	1.00	16.33
1943	CA	ASP	A	69	-13.077	-8.901	28.896	1.00	16.65
1944	C	ASP	A	69	-12.242	-7.625	28.717	1.00	16.41
1945	O	ASP	A	69	-12.564	-6.768	27.892	1.00	16.43
1946	CB	ASP	A	69	-14.15	-8.689	29.974	1.00	17.84
1947	CG	ASP	A	69	-15.212	-9.805	29.988	1.00	19.6
1948	OD1	ASP	A	69	-15.374	-10.51	28.96	1.00	20.42
1949	OD2	ASP	A	69	-15.901	-9.967	31.023	1.00	19.8
1950	N	LEU	A	70	-11.165	-7.507	29.486	1.00	15.9
1951	CA	LEU	A	70	-10.289	-6.35	29.379	1.00	15.89
1952	C	LEU	A	70	-9.577	-6.401	28.025	1.00	15.6
1953	O	LEU	A	70	-9.426	-5.382	27.357	1.00	15.63
1954	CB	LEU	A	70	-9.263	-6.348	30.516	1.00	16.17
1955	CG	LEU	A	70	-8.283	-5.173	30.494	1.00	16.78
1956	CD1	LEU	A	70	-9.05	-3.847	30.551	1.00	17.18
1957	CD2	LEU	A	70	-7.33	-5.286	31.674	1.00	17.17
1958	N	MET	A	71	-9.135	-7.596	27.631	1.00	15.23
1959	CA	MET	A	71	-8.471	-7.784	26.341	1.00	14.58



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TABLE 4

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

1960	C	MET	A	71	-9.409	-7.387	25.197	1.00	14.66
1961	O	MET	A	71	-9.003	-6.696	24.26	1.00	14.27
1962	CB	MET	A	71	-8.075	-9.25	26.146	1.00	14.17
1963	CG	MET	A	71	-6.966	-9.765	27.035	1.00	13.32
1964	SD	MET	A	71	-6.6	-11.484	26.595	1.00	12.96
1965	CE	MET	A	71	-6.19	-12.177	28.194	1.00	13.12
1966	N	ARG	A	72	-10.661	-7.835	25.285	1.00	14.94
1967	CA	ARG	A	72	-11.675	-7.559	24.268	1.00	15.66
1968	C	ARG	A	72	-11.963	-6.071	24.07	1.00	15.62
1969	O	ARG	A	72	-12.213	-5.634	22.947	1.00	15.61
1970	CB	ARG	A	72	-12.976	-8.3	24.604	1.00	16.6
1971	CG	ARG	A	72	-12.823	-9.823	24.637	1.00	17.97
1972	CD	ARG	A	72	-12.423	-10.366	23.269	1.00	19.29
1973	NE	ARG	A	72	-13.455	-10.086	22.27	1.00	20.82
1974	CZ	ARG	A	72	-14.105	-11.021	21.581	1.00	21.39
1975	NH1	ARG	A	72	-13.827	-12.307	21.772	1.00	21.4
1976	NH2	ARG	A	72	-15.049	-10.671	20.715	1.00	21.58
1977	N	GLN	A	73	-11.941	-5.293	25.149	1.00	15.43
1978	CA	GLN	A	73	-12.175	-3.853	25.023	1.00	15.53
1979	C	GLN	A	73	-11.058	-3.261	24.17	1.00	15.3
1980	O	GLN	A	73	-11.295	-2.387	23.338	1.00	15.36
1981	CB	GLN	A	73	-12.147	-3.152	26.384	1.00	15.72
1982	CG	GLN	A	73	-13.107	-3.68	27.429	1.00	16.61
1983	CD	GLN	A	73	-12.995	-2.919	28.746	1.00	17.45
1984	OE1	GLN	A	73	-13.258	-3.473	29.811	1.00	18.68
1985	NE2	GLN	A	73	-12.616	-1.643	28.676	1.00	17.08
1986	N	CYS	A	74	-9.835	-3.734	24.401	1.00	14.95
1987	CA	CYS	A	74	-8.676	-3.253	23.664	1.00	14.63
1988	C	CYS	A	74	-8.793	-3.493	22.166	1.00	14.51
1989	O	CYS	A	74	-8.203	-2.758	21.37	1.00	14.03
1990	CB	CYS	A	74	-7.398	-3.925	24.176	1.00	14.33
1991	SG	CYS	A	74	-6.932	-3.459	25.862	1.00	15.55
1992	N	TRP	A	75	-9.551	-4.518	21.777	1.00	14.46
1993	CA	TRP	A	75	-9.697	-4.836	20.358	1.00	14.74
1994	C	TRP	A	75	-11.012	-4.412	19.73	1.00	15.3
1995	O	TRP	A	75	-11.39	-4.933	18.679	1.00	15.63
1996	CB	TRP	A	75	-9.503	-6.337	20.114	1.00	13.63
1997	CG	TRP	A	75	-8.25	-6.878	20.693	1.00	13.09
1998	CD1	TRP	A	75	-7.009	-6.297	20.668	1.00	12.65
1999	CD2	TRP	A	75	-8.099	-8.12	21.386	1.00	12.82

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

2000	NE1	TRP	A	75	-6.098	-7.103	21.306	1.00	12.45
2001	CE2	TRP	A	75	-6.738	-8.227	21.758	1.00	12.47
2002	CE3	TRP	A	75	-8.98	-9.153	21.733	1.00	12.52
2003	CZ2	TRP	A	75	-6.239	-9.328	22.46	1.00	12.38
2004	CZ3	TRP	A	75	-8.481	-10.251	22.432	1.00	12.74
2005	CH2	TRP	A	75	-7.123	-10.326	22.787	1.00	12.45
2006	N	ARG	A	76	-11.723	-3.484	20.354	1.00	15.69
2007	CA	ARG	A	76	-12.973	-3.039	19.756	1.00	16.73
2008	C	ARG	A	76	-12.634	-2.465	18.389	1.00	17.4
2009	O	ARG	A	76	-11.601	-1.811	18.219	1.00	17.02
2010	CB	ARG	A	76	-13.645	-1.983	20.63	1.00	16.49
2011	CG	ARG	A	76	-14.231	-2.568	21.9	1.00	16.53
2012	CD	ARG	A	76	-14.661	-1.493	22.887	1.00	16.18
2013	NE	ARG	A	76	-15.273	-2.099	24.063	1.00	16.29
2014	CZ	ARG	A	76	-15.6	-1.439	25.169	1.00	16.33
2015	NH1	ARG	A	76	-16.155	-2.086	26.189	1.00	15.8
2016	NH2	ARG	A	76	-15.364	-0.136	25.258	1.00	16.57
2017	N	GLU	A	77	-13.499	-2.74	17.415	1.00	18.54
2018	CA	GLU	A	77	-13.317	-2.281	16.041	1.00	19.05
2019	C	GLU	A	77	-13.127	-0.771	15.961	1.00	18.61
2020	O	GLU	A	77	-12.178	-0.286	15.347	1.00	18.18
2021	CB	GLU	A	77	-14.526	-2.697	15.197	1.00	20.5
2022	CG	GLU	A	77	-14.426	-2.331	13.724	1.00	22.71
2023	CD	GLU	A	77	-15.628	-2.825	12.923	1.00	24.5
2024	OE1	GLU	A	77	-16.769	-2.406	13.23	1.00	25.43
2025	OE2	GLU	A	77	-15.43	-3.637	11.988	1.00	25.74
2026	N	LYS	A	78	-14.042	-0.032	16.575	1.00	18.47
2027	CA	LYS	A	78	-13.957	1.424	16.578	1.00	18.43
2028	C	LYS	A	78	-12.834	1.859	17.517	1.00	17.86
2029	O	LYS	A	78	-12.901	1.642	18.726	1.00	17.35
2030	CB	LYS	A	78	-15.289	2.024	17.027	1.00	19.21
2031	CG	LYS	A	78	-16.459	1.625	16.127	1.00	20.39
2032	CD	LYS	A	78	-17.757	2.29	16.569	1.00	21.98
2033	CE	LYS	A	78	-18.917	1.865	15.676	1.00	22.9
2034	NZ	LYS	A	78	-20.2	2.48	16.122	1.00	23.81
2035	N	PRO	A	79	-11.781	2.479	16.962	1.00	17.53
2036	CA	PRO	A	79	-10.628	2.947	17.74	1.00	17.23
2037	C	PRO	A	79	-10.992	3.785	18.964	1.00	17.42
2038	O	PRO	A	79	-10.442	3.569	20.042	1.00	17.29
2039	CB	PRO	A	79	-9.819	3.738	16.714	1.00	17.3

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## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

2040	CG	PRO	A	79	-10.109	3.002	15.421	1.00	17.51
2041	CD	PRO	A	79	-11.611	2.792	15.53	1.00	17.51
2042	N	TYR	A	80	-11.922	4.728	18.804	1.00	17.09
2043	CA	TYR	A	80	-12.306	5.586	19.918	1.00	17.31
2044	C	TYR	A	80	-13.153	4.94	21.005	1.00	16.94
2045	O	TYR	A	80	-13.412	5.561	22.033	1.00	17.29
2046	CB	TYR	A	80	-12.988	6.863	19.409	1.00	18.41
2047	CG	TYR	A	80	-12.003	7.845	18.813	1.00	19.62
2048	CD1	TYR	A	80	-11.942	8.059	17.437	1.00	20.7
2049	CD2	TYR	A	80	-11.082	8.513	19.624	1.00	20.54
2050	CE1	TYR	A	80	-10.981	8.916	16.879	1.00	21.25
2051	CE2	TYR	A	80	-10.118	9.364	19.084	1.00	20.89
2052	CZ	TYR	A	80	-10.072	9.561	17.711	1.00	21.46
2053	OH	TYR	A	80	-9.112	10.394	17.171	1.00	22.06
2054	N	GLU	A	81	-13.582	3.7	20.794	1.00	16.52
2055	CA	GLU	A	81	-14.369	3.01	21.806	1.00	16.02
2056	C	GLU	A	81	-13.443	2.215	22.733	1.00	15.95
2057	O	GLU	A	81	-13.861	1.732	23.793	1.00	15.9
2058	CB	GLU	A	81	-15.406	2.079	21.158	1.00	16.21
2059	CG	GLU	A	81	-16.498	2.8	20.351	1.00	16.38
2060	CD	GLU	A	81	-17.664	1.878	19.97	1.00	17.04
2061	OE1	GLU	A	81	-17.413	0.716	19.572	1.00	17.13
2062	OE2	GLU	A	81	-18.832	2.318	20.061	1.00	16.55
2063	N	ARG	A	82	-12.179	2.09	22.337	1.00	15.2
2064	CA	ARG	A	82	-11.208	1.37	23.145	1.00	14.96
2065	C	ARG	A	82	-10.914	2.164	24.417	1.00	14.69
2066	O	ARG	A	82	-11.04	3.385	24.441	1.00	15.06
2067	CB	ARG	A	82	-9.913	1.152	22.343	1.00	15.08
2068	CG	ARG	A	82	-10.118	0.268	21.119	1.00	14.81
2069	CD	ARG	A	82	-8.912	0.208	20.208	1.00	14.62
2070	NE	ARG	A	82	-9.315	-0.282	18.894	1.00	14.67
2071	CZ	ARG	A	82	-8.623	-0.093	17.773	1.00	15
2072	NH1	ARG	A	82	-7.47	0.568	17.801	1.00	14.54
2073	NH2	ARG	A	82	-9.117	-0.51	16.614	1.00	13.98
2074	N	PRO	A	83	-10.526	1.475	25.497	1.00	14.23
2075	CA	PRO	A	83	-10.231	2.203	26.734	1.00	13.98
2076	C	PRO	A	83	-8.894	2.934	26.617	1.00	13.72
2077	O	PRO	A	83	-8.114	2.688	25.693	1.00	13.78
2078	CB	PRO	A	83	-10.195	1.093	27.785	1.00	13.86
2079	CG	PRO	A	83	-9.621	-0.068	27.006	1.00	14.21

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

2080	CD	PRO	A	83	-10.348	0.021	25.673	1.00	14.01
2081	N	SER	A	84	-8.636	3.85	27.538	1.00	13.36
2082	CA	SER	A	84	-7.374	4.57	27.534	1.00	12.99
2083	C	SER	A	84	-6.453	3.748	28.425	1.00	12.74
2084	O	SER	A	84	-6.92	2.876	29.161	1.00	12.5
2085	CB	SER	A	84	-7.544	5.977	28.125	1.00	13.19
2086	OG	SER	A	84	-7.798	5.91	29.518	1.00	13.46
2087	N	PHE	A	85	-5.148	4.001	28.352	1.00	12.39
2088	CA	PHE	A	85	-4.228	3.261	29.195	1.00	12.11
2089	C	PHE	A	85	-4.56	3.549	30.661	1.00	11.85
2090	O	PHE	A	85	-4.416	2.681	31.517	1.00	11.62
2091	CB	PHE	A	85	-2.774	3.624	28.846	1.00	12.17
2092	CG	PHE	A	85	-2.263	2.905	27.627	1.00	11.86
2093	CD1	PHE	A	85	-2.098	1.523	27.647	1.00	11.81
2094	CD2	PHE	A	85	-2.009	3.591	26.442	1.00	11.76
2095	CE1	PHE	A	85	-1.693	0.83	26.505	1.00	11.69
2096	CE2	PHE	A	85	-1.603	2.907	25.289	1.00	11.74
2097	CZ	PHE	A	85	-1.446	1.523	25.324	1.00	11.65
2098	N	ALA	A	86	-5.044	4.755	30.938	1.00	11.96
2099	CA	ALA	A	86	-5.424	5.125	32.303	1.00	12.54
2100	C	ALA	A	86	-6.552	4.229	32.799	1.00	12.75
2101	O	ALA	A	86	-6.54	3.778	33.935	1.00	13.01
2102	CB	ALA	A	86	-5.872	6.59	32.356	1.00	12.26
2103	N	GLN	A	87	-7.534	3.979	31.941	1.00	13.17
2104	CA	GLN	A	87	-8.657	3.133	32.319	1.00	13.96
2105	C	GLN	A	87	-8.187	1.696	32.523	1.00	13.9
2106	O	GLN	A	87	-8.633	1.007	33.443	1.00	13.98
2107	CB	GLN	A	87	-9.749	3.209	31.246	1.00	14.48
2108	CG	GLN	A	87	-10.721	4.381	31.445	1.00	15.44
2109	CD	GLN	A	87	-11.184	4.999	30.137	1.00	16.41
2110	OE1	GLN	A	87	-11.235	4.329	29.107	1.00	16.41
2111	NE2	GLN	A	87	-11.536	6.289	30.174	1.00	16.72
2112	N	ILE	A	88	-7.275	1.258	31.666	1.00	13.66
2113	CA	ILE	A	88	-6.726	-0.089	31.751	1.00	13.51
2114	C	ILE	A	88	-5.961	-0.25	33.065	1.00	13.77
2115	O	ILE	A	88	-6.077	-1.273	33.726	1.00	14.2
2116	CB	ILE	A	88	-5.773	-0.369	30.563	1.00	12.94
2117	CG1	ILE	A	88	-6.583	-0.435	29.264	1.00	12.62
2118	CG2	ILE	A	88	-4.982	-1.657	30.805	1.00	12.19
2119	CD1	ILE	A	88	-5.725	-0.471	28.011	1.00	12.31

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

2120	N	LEU	A	89	-5.182	0.763	33.437	1.00	14.23
2121	CA	LEU	A	89	-4.411	0.713	34.68	1.00	14.68
2122	C	LEU	A	89	-5.335	0.608	35.895	1.00	15.04
2123	O	LEU	A	89	-5.067	-0.147	36.822	1.00	15.2
2124	CB	LEU	A	89	-3.516	1.954	34.821	1.00	14.18
2125	CG	LEU	A	89	-2.641	1.99	36.088	1.00	14.3
2126	CD1	LEU	A	89	-1.73	0.764	36.14	1.00	14.03
2127	CD2	LEU	A	89	-1.812	3.277	36.109	1.00	14.43
2128	N	VAL	A	90	-6.42	1.373	35.894	1.00	15.57
2129	CA	VAL	A	90	-7.367	1.316	36.999	1.00	16.21
2130	C	VAL	A	90	-7.943	-0.097	37.138	1.00	16.55
2131	O	VAL	A	90	-8.032	-0.626	38.242	1.00	16.73
2132	CB	VAL	A	90	-8.515	2.335	36.793	1.00	16.33
2133	CG1	VAL	A	90	-9.676	2.026	37.723	1.00	16.24
2134	CG2	VAL	A	90	-7.997	3.75	37.053	1.00	15.99
2135	N	SER	A	91	-8.331	-0.715	36.025	1.00	17.13
2136	CA	SER	A	91	-8.89	-2.067	36.084	1.00	17.74
2137	C	SER	A	91	-7.88	-3.08	36.616	1.00	17.97
2138	O	SER	A	91	-8.224	-3.935	37.437	1.00	17.38
2139	CB	SER	A	91	-9.374	-2.521	34.705	1.00	18.15
2140	OG	SER	A	91	-10.519	-1.787	34.303	1.00	19.38
2141	N	LEU	A	92	-6.64	-2.989	36.146	1.00	18.21
2142	CA	LEU	A	92	-5.611	-3.917	36.606	1.00	19.3
2143	C	LEU	A	92	-5.288	-3.71	38.087	1.00	20.11
2144	O	LEU	A	92	-5.101	-4.679	38.822	1.00	19.82
2145	CB	LEU	A	92	-4.339	-3.778	35.761	1.00	18.57
2146	CG	LEU	A	92	-4.48	-4.26	34.31	1.00	18.71
2147	CD1	LEU	A	92	-3.271	-3.851	33.489	1.00	18.13
2148	CD2	LEU	A	92	-4.653	-5.777	34.298	1.00	18.42
2149	N	ASN	A	93	-5.223	-2.456	38.531	1.00	21.26
2150	CA	ASN	A	93	-4.924	-2.198	39.94	1.00	22.76
2151	C	ASN	A	93	-5.981	-2.832	40.843	1.00	23.74
2152	O	ASN	A	93	-5.647	-3.352	41.904	1.00	23.78
2153	CB	ASN	A	93	-4.815	-0.688	40.224	1.00	22.51
2154	CG	ASN	A	93	-3.511	-0.081	39.698	1.00	22.47
2155	OD1	ASN	A	93	-2.548	-0.797	39.418	1.00	22.49
2156	ND2	ASN	A	93	-3.478	1.242	39.573	1.00	22.38
2157	N	ARG	A	94	-7.247	-2.8	40.42	1.00	25.08
2158	CA	ARG	A	94	-8.332	-3.397	41.207	1.00	26.6
2159	C	ARG	A	94	-8.142	-4.902	41.289	1.00	26.88

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

2160	O	ARG	A	94	-8.342	-5.507	42.338	1.00	26.8
2161	CB	ARG	A	94	-9.703	-3.128	40.584	1.00	27.72
2162	CG	ARG	A	94	-10.174	-1.688	40.623	1.00	29.81
2163	CD	ARG	A	94	-11.638	-1.611	40.187	1.00	31.6
2164	NE	ARG	A	94	-12.036	-0.255	39.823	1.00	33.23
2165	CZ	ARG	A	94	-13.241	0.076	39.368	1.00	34.01
2166	NH1	ARG	A	94	-13.511	1.343	39.059	1.00	34.39
2167	NH2	ARG	A	94	-14.18	-0.855	39.225	1.00	34.55
2168	N	MET	A	95	-7.773	-5.507	40.166	1.00	27.37
2169	CA	MET	A	95	-7.544	-6.939	40.131	1.00	28.03
2170	C	MET	A	95	-6.398	-7.302	41.084	1.00	28.42
2171	O	MET	A	95	-6.461	-8.308	41.795	1.00	28.09
2172	CB	MET	A	95	-7.228	-7.383	38.699	1.00	28.17
2173	CG	MET	A	95	-8.448	-7.353	37.772	1.00	28.73
2174	SD	MET	A	95	-8.125	-7.91	36.074	1.00	29.2
2175	CE	MET	A	95	-8.611	-6.492	35.165	1.00	28.75
2176	N	LEU	A	96	-5.366	-6.465	41.11	1.00	28.76
2177	CA	LEU	A	96	-4.221	-6.693	41.98	1.00	29.83
2178	C	LEU	A	96	-4.582	-6.553	43.455	1.00	30.8
2179	O	LEU	A	96	-3.951	-7.163	44.313	1.00	30.84
2180	CB	LEU	A	96	-3.092	-5.717	41.638	1.00	29.22
2181	CG	LEU	A	96	-2.327	-5.989	40.34	1.00	28.91
2182	CD1	LEU	A	96	-1.411	-4.814	40.019	1.00	28.66
2183	CD2	LEU	A	96	-1.535	-7.272	40.486	1.00	28.45
2184	N	GLU	A	97	-5.597	-5.745	43.743	1.00	32.19
2185	CA	GLU	A	97	-6.037	-5.519	45.117	1.00	33.72
2186	C	GLU	A	97	-6.94	-6.653	45.611	1.00	34.2
2187	O	GLU	A	97	-6.972	-6.955	46.807	1.00	34.14
2188	CB	GLU	A	97	-6.767	-4.173	45.217	1.00	34.71
2189	CG	GLU	A	97	-5.891	-2.965	44.884	1.00	36.14
2190	CD	GLU	A	97	-6.682	-1.661	44.823	1.00	37.55
2191	OE1	GLU	A	97	-7.391	-1.347	45.812	1.00	38.23
2192	OE2	GLU	A	97	-6.594	-0.948	43.791	1.00	37.84
2193	N	GLU	A	98	-7.673	-7.28	44.695	1.00	34.65
2194	CA	GLU	A	98	-8.549	-8.388	45.064	1.00	35.01
2195	C	GLU	A	98	-7.681	-9.608	45.364	1.00	35.06
2196	O	GLU	A	98	-6.564	-9.715	44.855	1.00	35.34
2197	CB	GLU	A	98	-9.51	-8.709	43.92	1.00	35.46
2198	CG	GLU	A	98	-10.425	-7.563	43.527	1.00	36.35
2199	CD	GLU	A	98	-11.306	-7.104	44.673	1.00	37.09

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## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

2200	OE1	GLU	A	98	-11.982	-7.963	45.286	1.00	37.2
2201	OE2	GLU	A	98	-11.323	-5.884	44.958	1.00	37.63
2202	N	ALA	A	99	-8.184	-10.526	46.183	1.00	34.89
2203	CA	ALA	A	99	-7.416	-11.72	46.528	1.00	35.03
2204	C	ALA	A	99	-7.615	-12.827	45.497	1.00	34.86
2205	O	ALA	A	99	-6.867	-13.807	45.466	1.00	35.11
2206	CB	ALA	A	99	-7.812	-12.22	47.922	1.00	35.35
2207	N	LYS	A	100	-8.624	-12.659	44.649	1.00	34.33
2208	CA	LYS	A	100	-8.936	-13.637	43.612	1.00	33.46
2209	C	LYS	A	100	-7.748	-13.924	42.688	1.00	32.45
2210	O	LYS	A	100	-6.88	-13.072	42.484	1.00	32.2
2211	CB	LYS	A	100	-10.118	-13.132	42.778	1.00	33.94
2212	CG	LYS	A	100	-10.508	-14.032	41.618	1.00	34.84
2213	CD	LYS	A	100	-11.682	-13.455	40.834	1.00	35.61
2214	CE	LYS	A	100	-12.142	-14.42	39.746	1.00	36.2
2215	NZ	LYS	A	100	-13.375	-13.962	39.041	1.00	36.65
2216	N	THR	A	101	-7.717	-15.138	42.144	1.00	31.1
2217	CA	THR	A	101	-6.678	-15.543	41.208	1.00	29.95
2218	C	THR	A	101	-7.251	-15.342	39.809	1.00	28.84
2219	O	THR	A	101	-8.19	-16.022	39.415	1.00	28.81
2220	CB	THR	A	101	-6.3	-17.029	41.395	1.00	30.34
2221	OG1	THR	A	101	-5.479	-17.17	42.561	1.00	30.79
2222	CG2	THR	A	101	-5.546	-17.552	40.182	1.00	30.54
2223	N	TYR	A	102	-6.696	-14.398	39.061	1.00	27.61
2224	CA	TYR	A	102	-7.191	-14.127	37.719	1.00	26.37
2225	C	TYR	A	102	-6.527	-14.968	36.64	1.00	25.84
2226	O	TYR	A	102	-7.178	-15.371	35.678	1.00	25.98
2227	CB	TYR	A	102	-7.035	-12.644	37.392	1.00	25.92
2228	CG	TYR	A	102	-7.841	-11.755	38.306	1.00	25.57
2229	CD1	TYR	A	102	-7.368	-11.415	39.575	1.00	25.27
2230	CD2	TYR	A	102	-9.102	-11.296	37.925	1.00	25.37
2231	CE1	TYR	A	102	-8.129	-10.644	40.444	1.00	25.28
2232	CE2	TYR	A	102	-9.878	-10.523	38.793	1.00	25.64
2233	CZ	TYR	A	102	-9.381	-10.205	40.052	1.00	25.65
2234	OH	TYR	A	102	-10.146	-9.471	40.926	1.00	26.19
2235	N	VAL	A	103	-5.235	-15.231	36.8	1.00	24.95
2236	CA	VAL	A	103	-4.5	-16.034	35.835	1.00	24.25
2237	C	VAL	A	103	-4.045	-17.338	36.49	1.00	23.92
2238	O	VAL	A	103	-3.048	-17.363	37.213	1.00	24.1
2239	CB	VAL	A	103	-3.264	-15.271	35.305	1.00	24.13

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TABLE 4

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

2240	CG1	VAL	A	103	-2.543	-16.107	34.263	1.00	23.85
2241	CG2	VAL	A	103	-3.693	-13.944	34.713	1.00	24
2242	N	ASN	A	104	-4.774	-18.418	36.232	1.00	23.31
2243	CA	ASN	A	104	-4.437	-19.715	36.81	1.00	23.01
2244	C	ASN	A	104	-3.13	-20.297	36.292	1.00	22.84
2245	O	ASN	A	104	-2.863	-20.286	35.093	1.00	22.59
2246	CB	ASN	A	104	-5.555	-20.726	36.551	1.00	22.72
2247	CG	ASN	A	104	-5.206	-22.117	37.055	1.00	22.85
2248	OD1	ASN	A	104	-4.935	-22.305	38.241	1.00	22.53
2249	ND2	ASN	A	104	-5.208	-23.099	36.152	1.00	22.64
2250	N	THR	A	105	-2.322	-20.809	37.213	1.00	22.77
2251	CA	THR	A	105	-1.057	-21.433	36.866	1.00	23.08
2252	C	THR	A	105	-0.955	-22.789	37.566	1.00	23.24
2253	O	THR	A	105	0.111	-23.402	37.599	1.00	23.34
2254	CB	THR	A	105	0.151	-20.551	37.275	1.00	23.18
2255	OG1	THR	A	105	0.097	-20.279	38.68	1.00	23.38
2256	CG2	THR	A	105	0.139	-19.236	36.511	1.00	22.7
2257	N	THR	A	106	-2.074	-23.253	38.123	1.00	23.23
2258	CA	THR	A	106	-2.113	-24.543	38.811	1.00	23.3
2259	C	THR	A	106	-2.599	-25.617	37.845	1.00	23.48
2260	O	THR	A	106	-3.52	-25.386	37.063	1.00	23.15
2261	CB	THR	A	106	-3.05	-24.504	40.037	1.00	23.33
2262	OG1	THR	A	106	-2.579	-23.519	40.965	1.00	23.29
2263	CG2	THR	A	106	-3.088	-25.873	40.723	1.00	23.01
2264	N	LEU	A	107	-1.986	-26.794	37.915	1.00	23.77
2265	CA	LEU	A	107	-2.326	-27.887	37.015	1.00	24.08
2266	C	LEU	A	107	-3.724	-28.496	37.148	1.00	24.58
2267	O	LEU	A	107	-4.426	-28.646	36.142	1.00	24.9
2268	CB	LEU	A	107	-1.263	-28.99	37.117	1.00	24.05
2269	CG	LEU	A	107	0.15	-28.561	36.699	1.00	24.42
2270	CD1	LEU	A	107	1.105	-29.745	36.791	1.00	24.35
2271	CD2	LEU	A	107	0.125	-28.015	35.267	1.00	24.13
2272	N	TYR	A	108	-4.138	-28.849	38.362	1.00	24.53
2273	CA	TYR	A	108	-5.456	-29.458	38.547	1.00	24.69
2274	C	TYR	A	108	-5.666	-30.636	37.582	1.00	24.69
2275	O	TYR	A	108	-4.764	-31.452	37.401	1.00	24.5
2276	CB	TYR	A	108	-6.55	-28.404	38.355	1.00	25.18
2277	CG	TYR	A	108	-6.587	-27.373	39.462	1.00	25.62
2278	CD1	TYR	A	108	-6.881	-26.043	39.189	1.00	25.64
2279	CD2	TYR	A	108	-6.347	-27.736	40.789	1.00	25.95



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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

2280	CE1	TYR	A	108	-6.936	-25.097	40.21	1.00	26.38
2281	CE2	TYR	A	108	-6.401	-26.8	41.816	1.00	26.25
2282	CZ	TYR	A	108	-6.696	-25.482	41.521	1.00	26.38
2283	OH	TYR	A	108	-6.751	-24.545	42.532	1.00	27.2
2284	N	GLU	A	109	-6.842	-30.722	36.959	1.00	24.8
2285	CA	GLU	A	109	-7.14	-31.822	36.035	1.00	25.01
2286	C	GLU	A	109	-6.576	-31.652	34.626	1.00	24.81
2287	O	GLU	A	109	-6.256	-32.64	33.958	1.00	24.77
2288	CB	GLU	A	109	-8.654	-32.033	35.886	1.00	25.65
2289	CG	GLU	A	109	-9.438	-32.283	37.164	1.00	26.73
2290	CD	GLU	A	109	-9.919	-30.997	37.82	1.00	27.4
2291	OE1	GLU	A	109	-10.114	-29.989	37.096	1.00	28.03
2292	OE2	GLU	A	109	-10.119	-30.998	39.053	1.00	27.06
2293	N	LYS	A	110	-6.461	-30.411	34.168	1.00	24.21
2294	CA	LYS	A	110	-5.992	-30.17	32.814	1.00	23.82
2295	C	LYS	A	110	-5.42	-28.766	32.624	1.00	23.14
2296	O	LYS	A	110	-5.92	-27.797	33.199	1.00	22.95
2297	CB	LYS	A	110	-7.168	-30.395	31.866	1.00	24.78
2298	CG	LYS	A	110	-6.896	-30.205	30.392	1.00	26.27
2299	CD	LYS	A	110	-8.183	-30.461	29.633	1.00	27.33
2300	CE	LYS	A	110	-8.056	-30.173	28.153	1.00	28.11
2301	NZ	LYS	A	110	-9.391	-30.352	27.515	1.00	29.1
2302	N	PHE	A	111	-4.365	-28.666	31.821	1.00	22.14
2303	CA	PHE	A	111	-3.732	-27.382	31.549	1.00	21.21
2304	C	PHE	A	111	-3.166	-27.377	30.137	1.00	20.83
2305	O	PHE	A	111	-2.612	-28.378	29.677	1.00	20.72
2306	CB	PHE	A	111	-2.616	-27.1	32.559	1.00	20.76
2307	CG	PHE	A	111	-2.142	-25.676	32.543	1.00	20.57
2308	CD1	PHE	A	111	-1.288	-25.221	31.54	1.00	20.55
2309	CD2	PHE	A	111	-2.6	-24.772	33.498	1.00	20.22
2310	CE1	PHE	A	111	-0.9	-23.884	31.484	1.00	20.53
2311	CE2	PHE	A	111	-2.219	-23.435	33.454	1.00	20.51
2312	CZ	PHE	A	111	-1.367	-22.986	32.443	1.00	20.53
2313	N	THR	A	112	-3.3	-26.245	29.455	1.00	20.19
2314	CA	THR	A	112	-2.822	-26.131	28.087	1.00	19.91
2315	C	THR	A	112	-1.854	-24.977	27.867	1.00	19.95
2316	O	THR	A	112	-2.057	-23.866	28.372	1.00	20
2317	CB	THR	A	112	-4.014	-25.983	27.115	1.00	19.94
2318	OG1	THR	A	112	-4.776	-27.197	27.113	1.00	19.78
2319	CG2	THR	A	112	-3.532	-25.691	25.699	1.00	19.65

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STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

2320	N	TYR	A	113	-0.797	-25.256	27.113	1.00	19.68
2321	CA	TYR	A	113	0.211	-24.255	26.782	1.00	19.98
2322	C	TYR	A	113	-0.038	-23.773	25.359	1.00	20.22
2323	O	TYR	A	113	-0.007	-24.568	24.419	1.00	19.76
2324	CB	TYR	A	113	1.614	-24.861	26.838	1.00	19.77
2325	CG	TYR	A	113	2.302	-24.831	28.183	1.00	19.85
2326	CD1	TYR	A	113	3.356	-25.702	28.447	1.00	20.03
2327	CD2	TYR	A	113	1.936	-23.917	29.178	1.00	19.56
2328	CE1	TYR	A	113	4.033	-25.673	29.658	1.00	20.22
2329	CE2	TYR	A	113	2.616	-23.882	30.405	1.00	19.79
2330	CZ	TYR	A	113	3.663	-24.769	30.628	1.00	19.97
2331	OH	TYR	A	113	4.357	-24.78	31.811	1.00	20.47
2332	N	ALA	A	114	-0.284	-22.477	25.199	1.00	20.51
2333	CA	ALA	A	114	-0.505	-21.918	23.874	1.00	20.89
2334	C	ALA	A	114	0.736	-22.199	23.024	1.00	21.41
2335	O	ALA	A	114	1.856	-22.229	23.537	1.00	20.94
2336	CB	ALA	A	114	-0.751	-20.416	23.973	1.00	20.6
2337	N	GLY	A	115	0.529	-22.412	21.729	1.00	22.09
2338	CA	GLY	A	115	1.638	-22.691	20.838	1.00	23.84
2339	C	GLY	A	115	2.618	-21.539	20.693	1.00	25.3
2340	O	GLY	A	115	2.238	-20.366	20.778	1.00	25.07
2341	N	ILE	A	116	3.885	-21.886	20.479	1.00	26.7
2342	CA	ILE	A	116	4.961	-20.918	20.307	1.00	28.74
2343	C	ILE	A	116	5.586	-21.056	18.913	1.00	30.06
2344	O	ILE	A	116	5.882	-20.057	18.257	1.00	30.32
2345	CB	ILE	A	116	6.06	-21.119	21.378	1.00	28.91
2346	CG1	ILE	A	116	5.551	-20.633	22.738	1.00	29.34
2347	CG2	ILE	A	116	7.329	-20.368	20.986	1.00	29.47
2348	CD1	ILE	A	116	6.535	-20.861	23.879	1.00	29.37
2349	N	ASP	A	117	5.789	-22.298	18.477	1.00	31.35
2350	CA	ASP	A	117	6.364	-22.588	17.165	1.00	32.9
2351	C	ASP	A	117	5.195	-22.737	16.206	1.00	33.47
2352	O	ASP	A	117	4.532	-23.774	16.171	1.00	33.69
2353	CB	ASP	A	117	7.182	-23.884	17.222	1.00	33.49
2354	CG	ASP	A	117	8.302	-23.816	18.245	1.00	34.1
2355	OD1	ASP	A	117	9.199	-22.961	18.08	1.00	34.51
2356	OD2	ASP	A	117	8.281	-24.602	19.218	1.00	34.39
2357	N	CYS	A	118	4.953	-21.694	15.421	1.00	34.14
2358	CA	CYS	A	118	3.825	-21.682	14.508	1.00	34.98
2359	C	CYS	A	118	4.211	-21.711	13.038	1.00	36.2

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TABLE 4  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

2360	O	CYS	A	118	4.325	-20.672	12.386	1.00	36.72
2361	CB	CYS	A	118	2.973	-20.453	14.836	1.00	33.87
2362	SG	CYS	A	118	2.916	-20.276	16.649	1.00	32.81
2363	N	ALA	A	119	4.411	-22.919	12.522	1.00	37.31
2364	CA	ALA	A	119	4.768	-23.105	11.12	1.00	38.2
2365	C	ALA	A	119	3.638	-23.859	10.429	1.00	38.7
2366	O	ALA	A	119	2.927	-23.233	9.611	1.00	39.14
2367	CB	ALA	A	119	6.075	-23.888	11.007	1.00	38.26
2368	OXT	ALA	A	119	3.466	-25.061	10.73	1.00	39.17
2369	O	HOH		1	30.621	13.917	26.008	1.00	25.56
2370	O	HOH		2	34.431	11.97	27.954	1.00	25.56
2371	O	HOH		3	39.022	2.328	27.593	1.00	59.58
2372	O	HOH		4	15.803	-7.852	23.714	1.00	13.06
2373	O	HOH		5	13.269	-8.599	22.276	1.00	22.7
2374	O	HOH		6	11.979	-5.585	19.53	1.00	22.53
2375	O	HOH		7	20.715	0.257	34.637	1.00	14.2
2376	O	HOH		8	11.295	-16.796	33.758	1.00	23.29
2377	O	HOH		9	10.355	-23.165	33.974	1.00	27.46
2378	O	HOH		10	-0.838	-18.279	40.306	1.00	30.3
2379	O	HOH		11	-1.211	-14.743	42.913	1.00	23.87
2380	O	HOH		12	-3.052	-20.626	40.135	1.00	24.53
2381	O	HOH		13	-5.425	-10.58	42.78	1.00	21.49
2382	O	HOH		14	6.385	-6.291	37.388	1.00	31.19
2383	O	HOH		15	-0.488	2.846	39.468	1.00	32.92
2384	O	HOH		16	-4.577	7.24	29.542	1.00	20.63
2385	O	HOH		17	0.177	1.579	17.372	1.00	14.69
2386	O	HOH		18	1.966	-0.566	19.733	1.00	12.31
2387	O	HOH		19	2.285	-2.83	15.996	1.00	20.53
2388	O	HOH		20	3.678	-4.723	17.995	1.00	21.9
2389	O	HOH		21	6.556	-10.331	21.736	1.00	17.54
2390	O	HOH		22	7.754	-11.797	19.48	1.00	21.28
2391	O	HOH		23	4.412	-13.933	21.512	1.00	14.92
2392	O	HOH		24	6.668	10.767	14.187	1.00	27.38
2393	O	HOH		25	-2.886	9.172	19.566	1.00	18.14
2394	O	HOH		26	2.986	0.158	8.786	1.00	21.09
2395	O	HOH		27	3.5	-10.726	13.238	1.00	7.11
2396	O	HOH		28	-3.873	-8.632	16.369	1.00	10.99
2397	O	HOH		29	-6.124	4.351	15.693	1.00	18.19
2398	O	HOH		30	-7.849	6.576	16.593	1.00	18.54
2399	O	HOH		31	-3.978	-3.095	3.842	1.00	23.51

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## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

2400	O	HOH		32	-11.384	0.244	6.226	1.00	43.39
2401	O	HOH		33	-7.503	-10.267	18.777	1.00	15.99
2402	O	HOH		34	-0.229	-19.365	20.767	1.00	19.65
2403	O	HOH		35	-2.999	-20.536	20.632	1.00	41.52
2404	O	HOH		36	-0.048	-21.104	27.564	1.00	15.32
2405	O	HOH		37	-4.951	-21.852	26.113	1.00	22.54
2406	O	HOH		38	-2.714	-20.092	27.945	1.00	26.38
2407	O	HOH		39	-5.266	-19.988	16.514	1.00	38.99
2408	O	HOH		40	-5.088	-24.24	30.831	1.00	17.34
2409	O	HOH		41	-6.212	-23.677	33.552	1.00	15.13
2410	O	HOH		42	-6.548	-26.567	29.923	1.00	23.67
2411	O	HOH		43	-5.445	-26.302	35.26	1.00	22.35
2412	O	HOH		44	-8.974	-18.306	35.861	1.00	36.13
2413	O	HOH		45	-12.561	-6.438	33.081	1.00	29.39
2414	O	HOH		46	-13.66	0.694	29.534	1.00	18.52
2415	O	HOH		47	-15.483	1.544	27.564	1.00	24.17
2416	O	HOH		48	-14.081	3.022	30.258	1.00	30.48
2417	O	HOH		49	-18.419	-1.343	21.665	1.00	31
2418	O	HOH		50	-15.799	-4.507	18.027	1.00	23.52
2419	O	HOH		51	-16.103	-1.028	18.213	1.00	14.42
2420	O	HOH		52	-12.016	7.86	23.37	1.00	19.74
2421	O	HOH		53	-10.35	5.376	22.682	1.00	16.34
2422	O	HOH		54	-11.799	5.22	26.375	1.00	25.97
2423	O	HOH		55	-9.119	6.055	34.294	1.00	27.46
2424	O	HOH		56	-11.144	1.669	34.441	1.00	22.08
2425	O	HOH		57	-2.434	-32.076	38.879	1.00	31.73
2426	O	HOH		58	31.02	10.062	34.12	1.00	26.26
2427	O	HOH		59	35.032	11.739	25.137	1.00	32.77
2428	O	HOH		60	35.513	3.746	27.996	1.00	18.32
2429	O	HOH		61	35.847	-0.913	28.564	1.00	25.92
2430	O	HOH		62	20.024	-10.654	25.05	1.00	51.68
2431	O	HOH		63	16.763	-10.331	21.864	1.00	55.99
2432	O	HOH		64	19.287	-4.341	29.331	1.00	24.82
2433	O	HOH		65	13.356	-8.06	19.495	1.00	36.59
2434	O	HOH		66	12.5	-11.507	21.419	1.00	35.31
2435	O	HOH		67	9.754	-5.726	16.927	1.00	23.49
2436	O	HOH		68	25.258	-0.307	20.133	1.00	36.17
2437	O	HOH		69	23.609	0.399	17.337	1.00	41.55
2438	O	HOH		70	23.12	-0.464	38.622	1.00	47.49
2439	O	HOH		71	23.392	8.194	13.714	1.00	41.63

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TABLE 4  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

2440	O	HOH		72	11.953	8.273	17.609	1.00	36.95
2441	O	HOH		73	11.883	7.088	21.028	1.00	24.4
2442	O	HOH		74	7.512	10.164	36.032	1.00	32.33
2443	O	HOH		75	10.561	8.488	37.605	1.00	38.68
2444	O	HOH		76	12.214	6.712	36.893	1.00	34.27
2445	O	HOH		77	6.776	0.016	38.787	1.00	28.27
2446	O	HOH		78	36.169	13.132	21.73	1.00	26.63
2447	O	HOH		79	34.857	6.677	19.799	1.00	24.5
2448	O	HOH		80	36.217	6.153	17.478	1.00	20.44
2449	O	HOH		81	16.502	-2.154	35.159	1.00	18.04
2450	O	HOH		82	14.218	-12.624	29.747	1.00	19.17
2451	O	HOH		83	5.93	-14.173	19.054	1.00	33.87
2452	O	HOH		84	7.7	-16.697	18.528	1.00	29.53
2453	O	HOH		85	14.062	-16.547	33.024	1.00	28.21
2454	O	HOH		86	11.04	-17.276	36.451	1.00	45.81
2455	O	HOH		87	6.811	-31.267	29.224	1.00	29.5
2456	O	HOH		88	2.61	-19.841	39.924	1.00	34.9
2457	O	HOH		89	-4.179	-12.505	41.019	1.00	25.96
2458	O	HOH		90	6.193	-9.214	38.671	1.00	33.53
2459	O	HOH		91	2.606	-3.017	38.954	1.00	23.05
2460	O	HOH		92	9.546	-10.928	42.605	1.00	43.3
2461	O	HOH		93	0.655	6.571	34.617	1.00	32.7
2462	O	HOH		94	2.693	6.896	36.804	1.00	33.29
2463	O	HOH		95	-3.517	7.642	35.197	1.00	26.45
2464	O	HOH		96	-5.078	5.431	36.121	1.00	27.83
2465	O	HOH		97	0.301	5.951	22.799	1.00	12.52
2466	O	HOH		98	-1.443	10.553	20.973	1.00	25.48
2467	O	HOH		99	8.581	1.149	17.855	1.00	32.27
2468	O	HOH		100	0.456	-1.233	17.155	1.00	21.68
2469	O	HOH		101	-1.411	-1.367	15.136	1.00	13.82
2470	O	HOH		102	6.185	1.375	12.771	1.00	45.72
2471	O	HOH		103	5.738	-0.985	13.576	1.00	33.56
2472	O	HOH		104	-2.073	-22.684	20.117	1.00	23.49
2473	O	HOH		105	-4.014	-17.857	19.118	1.00	21.06
2474	O	HOH		106	-4.357	-22.548	29.017	1.00	23.02
2475	O	HOH		107	-5.649	-21.241	40.508	1.00	26.85
2476	O	HOH		108	8.742	1.156	40.386	1.00	26.04
2477	O	HOH		109	-3.489	-8.116	14.062	1.00	16.19
2478	O	HOH		110	-10.445	-0.322	13.048	1.00	27.97
2479	O	HOH		111	-10.949	0.882	3.238	1.00	42.54

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TABLE 4  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

2480	O	HOH		112	-10.066	0.121	9.174	1.00	35.31
2481	O	HOH		113	-7.514	5.974	13.327	1.00	46.41
2482	O	HOH		114	-7.109	4.835	24.056	1.00	19.24
2483	O	HOH		115	-10.9	7.548	26.005	1.00	27.82
2484	O	HOH		116	-4.415	5.454	25.633	1.00	32.9
2485	O	HOH		117	-6.649	-17.491	16.708	1.00	31.38
2486	O	HOH		118	-14.016	-6.067	13.748	1.00	24.34
2487	O	HOH		119	-13.187	-7.475	21	1.00	17.13
2488	O	HOH		120	-14.926	-6.739	19.143	1.00	40.99
2489	O	HOH		121	-13.548	-16.943	34.739	1.00	34.53
2490	O	HOH		122	-15.436	-15.677	36.048	1.00	44.01
2491	O	HOH		123	-12.194	-8.527	39.864	1.00	48.62
2492	O	HOH		124	9.249	-19.53	17.927	1.00	34.18
2493	O	HOH		125	1.83	-22.29	39.943	1.00	34.34
2494	O	HOH		126	0.404	-23.193	41.823	1.00	36.15
2495	O	HOH		127	13.074	-25.67	34.335	1.00	43.38
2496	O	HOH		128	12.465	-23.322	36.118	1.00	34.43
2497	O	HOH		129	13.877	-13.365	22.591	1.00	41.93
2498	O	HOH		130	15.506	-11.967	26.529	1.00	39.81
2499	O	HOH		131	20.082	-2.098	36.158	1.00	32.05
2500	O	HOH		132	-10.796	-0.607	31.26	1.00	33.1
2501	O	HOH		133	-11.208	4.313	34.821	1.00	31.64
2502	O	HOH		134	-7.641	7.408	36.256	1.00	30.18
2503	O	HOH		135	-10.217	7.751	32.72	1.00	30.89
2504	O	HOH		136	-8.878	8.335	30.442	1.00	27.73
2505	O	HOH		137	-6.102	9.401	30.388	1.00	28.72
2506	O	HOH		138	-13.859	5.282	16.507	1.00	16.29
2507	O	HOH		139	-16.3	-5.034	24.97	1.00	37.83
2508	O	HOH		140	-12.512	-17.412	23.727	1.00	30.95
2509	O	HOH		141	-6.729	-17.735	19.392	1.00	36.59
2510	O	HOH		142	-7.463	-20.22	20.013	1.00	34.67
2511	O	HOH		143	-11.12	-4.085	7.458	1.00	34.84
2512	O	HOH		144	-8.204	-6.321	7.356	1.00	42.15
2513	O	HOH		145	-0.55	-22.433	10.134	1.00	44.22
2514	O	HOH		146	0.928	-1.171	7.388	1.00	25.5
2515	O	HOH		147	7.525	-9.088	13.919	1.00	40.17
2516	O	HOH		148	7.551	-11.238	15.42	1.00	43.48
2517	O	HOH		149	10.867	2.045	17.252	1.00	36.51
2518	O	HOH		150	40.562	10.438	22.843	1.00	38.24
2519	O	HOH		151	27.468	-1.515	18.726	1.00	33.9

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TABLE 4  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM III

2520	O	HOH		152	27.47	2.304	15.706	1.00	40.91
2521	O	HOH		153	20.708	-2.716	16.608	1.00	38.73
2522	O	HOH		154	29.446	11.095	35.881	1.00	38.17
2523	O	HOH		155	5.497	2.72	39.356	1.00	28.81
2524	O	HOH		156	1.361	5.907	39.489	1.00	42.1
2525	O	HOH		157	3.766	-1.603	41.474	1.00	32.37
2526	O	HOH		158	5.98	-1.982	39.924	1.00	35.51
2527	O	HOH		159	11.597	1.183	39.041	1.00	34.97
2528	O	HOH		160	2.521	11.847	31.108	1.00	26.91
2529	O	HOH		161	14.103	7.811	19.536	1.00	38.25
2530	O	HOH		162	10.175	-1.603	17.077	1.00	36.61
2531	O	HOH		163	-13.048	-2.415	32.798	1.00	29.91
2532	O	HOH		164	-8.057	7.633	24.712	1.00	31.89
2533	O	HOH		165	16.607	-13.841	35.679	1.00	32.35
2534	O	HOH		166	30.282	2.018	12.942	1.00	38.83
2535	O	HOH		167	33.213	9.608	12.652	1.00	40.22
2536	O	HOH		168	3.936	-19.246	41.958	1.00	33.36
2537	O	HOH		169	1.686	-18.362	44.637	1.00	37.77
2538	O	HOH		170	0.396	-14.273	45.402	1.00	34.03

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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

ATOM	ATOM TYPE	RESIDUE	PROTEIN #	#	X	Y	Z	OCC	B
1	N	PRO	A	813	16.125	47.577	18.265	1.00	64.47
2	CA	PRO	A	813	15.107	46.54	18.571	1.00	64.29
3	C	PRO	A	813	13.966	47.136	19.392	1.00	64.15
4	O	PRO	A	813	14.188	48.027	20.215	1.00	64.32
5	CB	PRO	A	813	15.82	45.441	19.344	1.00	64.24
6	CG	PRO	A	813	16.953	46.231	20.003	1.00	64.38
7	CD	PRO	A	813	17.395	47.252	18.939	1.00	64.33
8	N	THR	A	814	12.748	46.646	19.165	1.00	63.67
9	CA	THR	A	814	11.574	47.142	19.884	1.00	62.92
10	C	THR	A	814	10.751	46.013	20.514	1.00	62.5
11	O	THR	A	814	10.621	44.926	19.946	1.00	62.31
12	CB	THR	A	814	10.657	47.975	18.956	1.00	63.18
13	OG1	THR	A	814	10.231	47.168	17.853	1.00	63.26
14	CG2	THR	A	814	11.402	49.196	18.426	1.00	62.95
15	N	ILE	A	815	10.193	46.283	21.69	1.00	61.56
16	CA	ILE	A	815	9.396	45.296	22.412	1.00	60.73
17	C	ILE	A	815	7.9	45.467	22.15	1.00	60.39
18	O	ILE	A	815	7.369	46.576	22.229	1.00	60.21
19	CB	ILE	A	815	9.647	45.399	23.937	1.00	60.69
20	CG1	ILE	A	815	11.134	45.178	24.239	1.00	60.73
21	CG2	ILE	A	815	8.791	44.385	24.68	1.00	60.42
22	CD1	ILE	A	815	11.659	43.811	23.849	1.00	60.85
23	N	TYR	A	816	7.225	44.36	21.849	1.00	59.55
24	CA	TYR	A	816	5.792	44.385	21.585	1.00	58.9
25	C	TYR	A	816	5.016	43.593	22.636	1.00	57.89
26	O	TYR	A	816	5.564	42.708	23.29	1.00	57.81
27	CB	TYR	A	816	5.494	43.806	20.201	1.00	59.73
28	CG	TYR	A	816	6.326	44.4	19.094	1.00	60.64
29	CD1	TYR	A	816	7.638	43.975	18.877	1.00	61.12
30	CD2	TYR	A	816	5.809	45.396	18.265	1.00	60.9
31	CE1	TYR	A	816	8.413	44.525	17.86	1.00	61.25
32	CE2	TYR	A	816	6.579	45.952	17.247	1.00	61.18
33	CZ	TYR	A	816	7.878	45.511	17.05	1.00	61.38
34	OH	TYR	A	816	8.643	46.052	16.039	1.00	62.02
35	N	PRO	A	817	3.725	43.912	22.814	1.00	56.97
36	CA	PRO	A	817	3.029	44.963	22.068	1.00	56.19
37	C	PRO	A	817	3.408	46.341	22.596	1.00	55.4
38	O	PRO	A	817	3.837	46.476	23.742	1.00	55.27
39	CB	PRO	A	817	1.562	44.634	22.308	1.00	56.24



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TABLE 5  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

40	CG	PRO	A	817	1.582	44.103	23.704	1.00	56.49
41	CD	PRO	A	817	2.785	43.184	23.684	1.00	56.72
42	N	VAL	A	818	3.256	47.359	21.756	1.00	54.36
43	CA	VAL	A	818	3.579	48.722	22.153	1.00	53.31
44	C	VAL	A	818	2.542	49.212	23.157	1.00	52.27
45	O	VAL	A	818	1.34	49.057	22.946	1.00	51.92
46	CB	VAL	A	818	3.586	49.668	20.94	1.00	53.66
47	CG1	VAL	A	818	4.029	51.063	21.369	1.00	53.59
48	CG2	VAL	A	818	4.504	49.111	19.859	1.00	53.58
49	N	LEU	A	819	3.011	49.796	24.254	1.00	51.29
50	CA	LEU	A	819	2.114	50.3	25.284	1.00	50.59
51	C	LEU	A	819	2.034	51.815	25.239	1.00	50.3
52	O	LEU	A	819	3.052	52.489	25.087	1.00	50.39
53	CB	LEU	A	819	2.6	49.871	26.672	1.00	50.41
54	CG	LEU	A	819	2.63	48.374	26.978	1.00	50.24
55	CD1	LEU	A	819	3.138	48.157	28.395	1.00	49.66
56	CD2	LEU	A	819	1.233	47.792	26.815	1.00	50.14
57	N	ASP	A	820	0.824	52.35	25.359	1.00	49.7
58	CA	ASP	A	820	0.656	53.795	25.36	1.00	49.4
59	C	ASP	A	820	0.905	54.283	26.774	1.00	48.68
60	O	ASP	A	820	0.396	53.712	27.741	1.00	48.71
61	CB	ASP	A	820	-0.755	54.202	24.924	1.00	50.13
62	CG	ASP	A	820	-1.01	53.948	23.452	1.00	50.97
63	OD1	ASP	A	820	-0.165	54.339	22.615	1.00	51.47
64	OD2	ASP	A	820	-2.066	53.367	23.132	1.00	51.64
65	N	TRP	A	821	1.693	55.343	26.883	1.00	47.51
66	CA	TRP	A	821	2.034	55.923	28.167	1.00	46.78
67	C	TRP	A	821	0.833	56.276	29.046	1.00	47.01
68	O	TRP	A	821	0.908	56.176	30.272	1.00	46.5
69	CB	TRP	A	821	2.891	57.166	27.941	1.00	45.33
70	CG	TRP	A	821	3.213	57.901	29.188	1.00	44.07
71	CD1	TRP	A	821	2.508	58.928	29.741	1.00	43.47
72	CD2	TRP	A	821	4.329	57.666	30.052	1.00	43.56
73	NE1	TRP	A	821	3.117	59.352	30.895	1.00	43.19
74	CE2	TRP	A	821	4.239	58.595	31.11	1.00	43.14
75	CE3	TRP	A	821	5.4	56.76	30.033	1.00	42.99
76	CZ2	TRP	A	821	5.177	58.647	32.143	1.00	42.67
77	CZ3	TRP	A	821	6.333	56.811	31.058	1.00	42.57
78	CH2	TRP	A	821	6.215	57.75	32.1	1.00	42.81
79	N	ASN	A	822	-0.272	56.681	28.428	1.00	47.49

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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

80	CA	ASN	A	822	-1.454	57.065	29.193	1.00	48.4
81	C	ASN	A	822	-2.24	55.891	29.771	1.00	48.24
82	O	ASN	A	822	-3.214	56.093	30.495	1.00	48.33
83	CB	ASN	A	822	-2.384	57.935	28.34	1.00	49.52
84	CG	ASN	A	822	-3.072	57.152	27.238	1.00	51.08
85	OD1	ASN	A	822	-2.42	56.531	26.397	1.00	52.18
86	ND2	ASN	A	822	-4.4	57.181	27.236	1.00	51.69
87	N	ASP	A	823	-1.826	54.668	29.451	1.00	47.82
88	CA	ASP	A	823	-2.504	53.487	29.98	1.00	47.12
89	C	ASP	A	823	-1.743	52.934	31.178	1.00	46.24
90	O	ASP	A	823	-2.213	52.026	31.866	1.00	46.59
91	CB	ASP	A	823	-2.621	52.403	28.911	1.00	47.28
92	CG	ASP	A	823	-3.576	52.785	27.805	1.00	47.91
93	OD1	ASP	A	823	-4.628	53.385	28.121	1.00	48.11
94	OD2	ASP	A	823	-3.284	52.475	26.629	1.00	47.89
95	N	ILE	A	824	-0.567	53.498	31.424	1.00	44.84
96	CA	ILE	A	824	0.271	53.067	32.529	1.00	43.7
97	C	ILE	A	824	0.035	53.907	33.775	1.00	43.22
98	O	ILE	A	824	0.118	55.134	33.734	1.00	43.7
99	CB	ILE	A	824	1.752	53.168	32.161	1.00	43.13
100	CG1	ILE	A	824	2.021	52.39	30.874	1.00	43.12
101	CG2	ILE	A	824	2.596	52.636	33.299	1.00	43.47
102	CD1	ILE	A	824	3.445	52.508	30.379	1.00	43.49
103	N	LYS	A	825	-0.264	53.238	34.881	1.00	42.35
104	CA	LYS	A	825	-0.488	53.912	36.149	1.00	41.2
105	C	LYS	A	825	0.585	53.448	37.12	1.00	40.28
106	O	LYS	A	825	0.579	52.297	37.559	1.00	40.01
107	CB	LYS	A	825	-1.871	53.569	36.702	1.00	42.31
108	CG	LYS	A	825	-2.153	54.168	38.068	1.00	43.97
109	CD	LYS	A	825	-3.595	53.924	38.497	1.00	45.72
110	CE	LYS	A	825	-3.896	54.609	39.826	1.00	46.62
111	NZ	LYS	A	825	-5.344	54.531	40.191	1.00	47.82
112	N	PHE	A	826	1.511	54.341	37.449	1.00	38.82
113	CA	PHE	A	826	2.588	54.001	38.364	1.00	37.65
114	C	PHE	A	826	2.105	54.091	39.799	1.00	37.2
115	O	PHE	A	826	1.461	55.064	40.185	1.00	37.41
116	CB	PHE	A	826	3.782	54.921	38.132	1.00	37.2
117	CG	PHE	A	826	4.29	54.893	36.72	1.00	37.15
118	CD1	PHE	A	826	3.724	55.709	35.746	1.00	36.54
119	CD2	PHE	A	826	5.311	54.019	36.352	1.00	36.97

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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

120	CE1	PHE	A	826	4.166	55.654	34.427	1.00	36.79
121	CE2	PHE	A	826	5.759	53.957	35.035	1.00	37.07
122	CZ	PHE	A	826	5.185	54.776	34.07	1.00	36.83
123	N	GLN	A	827	2.423	53.07	40.589	1.00	36.58
124	CA	GLN	A	827	1.979	53.014	41.971	1.00	35.8
125	C	GLN	A	827	3.081	53.026	43.014	1.00	35.03
126	O	GLN	A	827	2.952	53.698	44.031	1.00	34.86
127	CB	GLN	A	827	1.126	51.77	42.181	1.00	36.41
128	CG	GLN	A	827	0.213	51.45	41.013	1.00	37.56
129	CD	GLN	A	827	-0.626	50.218	41.266	1.00	38.02
130	OE1	GLN	A	827	-1.609	50.267	42.003	1.00	38.74
131	NE2	GLN	A	827	-0.232	49.099	40.669	1.00	37.88
132	N	ASP	A	828	4.161	52.286	42.782	1.00	34.29
133	CA	ASP	A	828	5.228	52.249	43.774	1.00	33.48
134	C	ASP	A	828	6.556	51.729	43.239	1.00	32.37
135	O	ASP	A	828	6.687	51.407	42.065	1.00	31.54
136	CB	ASP	A	828	4.792	51.386	44.958	1.00	34.34
137	CG	ASP	A	828	5.291	51.916	46.286	1.00	35.35
138	OD1	ASP	A	828	6.452	52.37	46.357	1.00	35.62
139	OD2	ASP	A	828	4.517	51.867	47.265	1.00	36.49
140	N	VAL	A	829	7.541	51.654	44.124	1.00	31.97
141	CA	VAL	A	829	8.863	51.173	43.759	1.00	31.7
142	C	VAL	A	829	9.146	49.884	44.522	1.00	30.74
143	O	VAL	A	829	9.04	49.838	45.744	1.00	30.82
144	CB	VAL	A	829	9.95	52.21	44.104	1.00	31.93
145	CG1	VAL	A	829	11.272	51.805	43.473	1.00	31.86
146	CG2	VAL	A	829	9.524	53.591	43.623	1.00	32.34
147	N	ILE	A	830	9.495	48.833	43.794	1.00	29.82
148	CA	ILE	A	830	9.782	47.547	44.411	1.00	28.6
149	C	ILE	A	830	10.978	46.901	43.733	1.00	27.99
150	O	ILE	A	830	11.476	47.395	42.727	1.00	28.22
151	CB	ILE	A	830	8.586	46.597	44.277	1.00	28.41
152	CG1	ILE	A	830	8.284	46.357	42.792	1.00	28.88
153	CG2	ILE	A	830	7.374	47.186	44.982	1.00	28.69
154	CD1	ILE	A	830	7.12	45.423	42.535	1.00	29.07
155	N	GLY	A	831	11.445	45.796	44.295	1.00	27.3
156	CA	GLY	A	831	12.566	45.103	43.7	1.00	26.03
157	C	GLY	A	831	12.024	43.886	42.99	1.00	25.46
158	O	GLY	A	831	10.96	43.38	43.348	1.00	25.14
159	N	GLU	A	832	12.729	43.42	41.97	1.00	25.33

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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

160	CA	GLU	A	832	12.283	42.234	41.259	1.00	24.9
161	C	GLU	A	832	13.449	41.424	40.7	1.00	24.77
162	O	GLU	A	832	13.742	41.47	39.503	1.00	24.72
163	CB	GLU	A	832	11.311	42.606	40.137	1.00	24.94
164	CG	GLU	A	832	10.625	41.381	39.562	1.00	25.5
165	CD	GLU	A	832	9.383	41.694	38.76	1.00	26.33
166	OE1	GLU	A	832	8.73	42.72	39.033	1.00	26
167	OE2	GLU	A	832	9.048	40.892	37.863	1.00	27.27
168	N	GLY	A	833	14.11	40.674	41.578	1.00	24.69
169	CA	GLY	A	833	15.234	39.858	41.153	1.00	24.67
170	C	GLY	A	833	16.318	40.662	40.46	1.00	24.64
171	O	GLY	A	833	16.65	41.764	40.898	1.00	24.68
172	N	ASN	A	834	16.866	40.128	39.372	1.00	24.16
173	CA	ASN	A	834	17.931	40.825	38.66	1.00	24.03
174	C	ASN	A	834	17.458	41.992	37.798	1.00	24.48
175	O	ASN	A	834	18.243	42.59	37.066	1.00	24.39
176	CB	ASN	A	834	18.773	39.831	37.842	1.00	22.59
177	CG	ASN	A	834	17.938	38.934	36.94	1.00	22.45
178	OD1	ASN	A	834	18.395	37.862	36.529	1.00	22.85
179	ND2	ASN	A	834	16.729	39.366	36.615	1.00	19.36
180	N	PHE	A	835	16.172	42.315	37.883	1.00	24.68
181	CA	PHE	A	835	15.644	43.455	37.153	1.00	25.53
182	C	PHE	A	835	15.988	44.686	37.996	1.00	25.69
183	O	PHE	A	835	15.898	45.815	37.537	1.00	26.52
184	CB	PHE	A	835	14.119	43.366	36.994	1.00	25.43
185	CG	PHE	A	835	13.662	42.487	35.854	1.00	25.86
186	CD1	PHE	A	835	13.356	41.144	36.062	1.00	25.51
187	CD2	PHE	A	835	13.513	43.013	34.572	1.00	25.62
188	CE1	PHE	A	835	12.904	40.338	35.008	1.00	25.53
189	CE2	PHE	A	835	13.062	42.216	33.511	1.00	25.65
190	CZ	PHE	A	835	12.758	40.878	33.732	1.00	25.37
191	N	GLY	A	836	16.391	44.451	39.239	1.00	26.7
192	CA	GLY	A	836	15.724	45.541	40.135	1.00	26.75
193	C	GLY	A	836	15.456	46.199	40.637	1.00	27.78
194	O	GLY	A	836	14.435	45.533	40.841	1.00	27.72
195	N	GLN	A	837	15.51	47.509	40.839	1.00	28.19
196	CA	GLN	A	837	14.345	48.246	41.303	1.00	28.64
197	C	GLN	A	837	13.43	48.519	40.119	1.00	28.28
198	O	GLN	A	837	13.879	48.984	39.074	1.00	28.41
199	CB	GLN	A	837	14.774	49.566	41.945	1.00	29.77

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TABLE 5  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

200	CG	GLN	A	837	15.525	49.39	43.247	1.00	31.16
201	CD	GLN	A	837	14.637	48.865	44.358	1.00	33.09
202	OE1	GLN	A	837	13.731	49.558	44.822	1.00	34.29
203	NE2	GLN	A	837	14.886	47.632	44.787	1.00	33.68
204	N	VAL	A	838	12.15	48.212	40.284	1.00	27.91
205	CA	VAL	A	838	11.172	48.434	39.233	1.00	28.28
206	C	VAL	A	838	9.977	49.189	39.81	1.00	28.66
207	O	VAL	A	838	9.89	49.398	41.016	1.00	28.36
208	CB	VAL	A	838	10.715	47.095	38.601	1.00	27.99
209	CG1	VAL	A	838	11.901	46.414	37.922	1.00	28.23
210	CG2	VAL	A	838	10.138	46.183	39.659	1.00	27.41
211	N	LEU	A	839	9.06	49.602	38.943	1.00	29.74
212	CA	LEU	A	839	7.893	50.361	39.373	1.00	30.35
213	C	LEU	A	839	6.615	49.538	39.337	1.00	30.99
214	O	LEU	A	839	6.178	49.117	38.272	1.00	30.74
215	CB	LEU	A	839	7.728	51.583	38.471	1.00	30.22
216	CG	LEU	A	839	9.003	52.406	38.25	1.00	30.86
217	CD1	LEU	A	839	8.776	53.418	37.145	1.00	30.75
218	CD2	LEU	A	839	9.406	53.091	39.548	1.00	30.47
219	N	LYS	A	840	6.019	49.303	40.501	1.00	32.01
220	CA	LYS	A	840	4.776	48.552	40.555	1.00	33.71
221	C	LYS	A	840	3.757	49.433	39.852	1.00	34.71
222	O	LYS	A	840	3.631	50.619	40.162	1.00	34.71
223	CB	LYS	A	840	4.349	48.307	42.002	1.00	34.04
224	CG	LYS	A	840	3.067	47.495	42.13	1.00	35.21
225	CD	LYS	A	840	2.709	47.262	43.587	1.00	36.9
226	CE	LYS	A	840	1.414	46.48	43.715	1.00	37.61
227	NZ	LYS	A	840	0.276	47.195	43.061	1.00	39.2
228	N	ALA	A	841	3.032	48.862	38.901	1.00	35.65
229	CA	ALA	A	841	2.058	49.642	38.164	1.00	37.15
230	C	ALA	A	841	0.881	48.816	37.685	1.00	38.43
231	O	ALA	A	841	0.794	47.611	37.932	1.00	38.8
232	CB	ALA	A	841	2.735	50.302	36.971	1.00	36.5
233	N	ARG	A	842	-0.034	49.497	37.011	1.00	39.65
234	CA	ARG	A	842	-1.2	48.866	36.432	1.00	41.73
235	C	ARG	A	842	-1.166	49.318	34.985	1.00	42.59
236	O	ARG	A	842	-0.962	50.496	34.705	1.00	42.79
237	CB	ARG	A	842	-2.48	49.352	37.111	1.00	42.32
238	CG	ARG	A	842	-2.588	48.979	38.578	1.00	43.77
239	CD	ARG	A	842	-3.953	48.392	38.872	1.00	46.25

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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

240	NE	ARG	A	842	-4.162	47.148	38.132	1.00	48.28
241	CZ	ARG	A	842	-5.291	46.445	38.133	1.00	48.9
242	NH1	ARG	A	842	-6.339	46.856	38.833	1.00	49.19
243	NH2	ARG	A	842	-5.367	45.318	37.438	1.00	49.29
244	N	ILE	A	843	-1.328	48.383	34.061	1.00	43.74
245	CA	ILE	A	843	-1.307	48.742	32.659	1.00	45.44
246	C	ILE	A	843	-2.552	48.223	31.967	1.00	47.39
247	O	ILE	A	843	-3.334	47.467	32.545	1.00	47.41
248	CB	ILE	A	843	-0.061	48.18	31.941	1.00	44.83
249	CG1	ILE	A	843	-0.111	46.651	31.91	1.00	44.65
250	CG2	ILE	A	843	1.2	48.653	32.648	1.00	44.63
251	CD1	ILE	A	843	0.998	46.021	31.087	1.00	43.34
252	N	LYS	A	844	-2.728	48.644	30.723	1.00	49.6
253	CA	LYS	A	844	-3.871	48.234	29.929	1.00	51.97
254	C	LYS	A	844	-3.357	47.577	28.659	1.00	53.26
255	O	LYS	A	844	-2.924	48.251	27.726	1.00	53.54
256	CB	LYS	A	844	-4.732	49.452	29.589	1.00	52.41
257	CG	LYS	A	844	-5.976	49.151	28.779	1.00	53.51
258	CD	LYS	A	844	-6.725	50.44	28.461	1.00	54.5
259	CE	LYS	A	844	-7.891	50.195	27.514	1.00	55.3
260	NZ	LYS	A	844	-8.561	51.466	27.109	1.00	56.12
261	N	LYS	A	845	-3.378	46.251	28.648	1.00	54.95
262	CA	LYS	A	845	-2.934	45.486	27.492	1.00	56.53
263	C	LYS	A	845	-4.213	45.098	26.756	1.00	57.32
264	O	LYS	A	845	-5.104	44.465	27.331	1.00	57.46
265	CB	LYS	A	845	-2.165	44.244	27.95	1.00	56.62
266	CG	LYS	A	845	-1.34	43.57	26.869	1.00	56.99
267	CD	LYS	A	845	-0.561	42.395	27.437	1.00	56.79
268	CE	LYS	A	845	0.242	41.691	26.358	1.00	57.01
269	NZ	LYS	A	845	0.902	40.469	26.887	1.00	57.04
270	N	ASP	A	846	-4.304	45.483	25.488	1.00	58.22
271	CA	ASP	A	846	-5.501	45.207	24.709	1.00	58.95
272	C	ASP	A	846	-6.622	46.043	25.319	1.00	58.89
273	O	ASP	A	846	-6.762	47.223	24.998	1.00	59.54
274	CB	ASP	A	846	-5.856	43.72	24.763	1.00	59.85
275	CG	ASP	A	846	-4.924	42.868	23.925	1.00	60.86
276	OD1	ASP	A	846	-3.692	42.95	24.128	1.00	61.44
277	OD2	ASP	A	846	-5.428	42.114	23.063	1.00	61.46
278	N	GLY	A	847	-7.404	45.445	26.212	1.00	58.45
279	CA	GLY	A	847	-8.486	46.19	26.83	1.00	57.58

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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

280	C	GLY	A	847	-8.79	45.792	28.26	1.00	56.95
281	O	GLY	A	847	-9.954	45.748	28.655	1.00	57.29
282	N	LEU	A	848	-7.756	45.505	29.045	1.00	56.28
283	CA	LEU	A	848	-7.966	45.113	30.434	1.00	55.23
284	C	LEU	A	848	-6.957	45.763	31.374	1.00	53.87
285	O	LEU	A	848	-5.805	45.966	31.019	1.00	53.64
286	CB	LEU	A	848	-7.918	43.579	30.553	1.00	56.05
287	CG	LEU	A	848	-6.802	42.842	31.303	1.00	56.39
288	CD1	LEU	A	848	-6.944	43.053	32.804	1.00	57.01
289	CD2	LEU	A	848	-6.887	41.359	30.988	1.00	56.52
290	N	ARG	A	849	-7.409	46.104	32.574	1.00	52.68
291	CA	ARG	A	849	-6.547	46.722	33.574	1.00	51.49
292	C	ARG	A	849	-5.869	45.625	34.398	1.00	50.02
293	O	ARG	A	849	-6.522	44.94	35.187	1.00	50.16
294	CB	ARG	A	849	-7.377	47.633	34.482	1.00	52.09
295	CG	ARG	A	849	-8.014	48.811	33.755	1.00	53.19
296	CD	ARG	A	849	-6.955	49.795	33.296	1.00	54.07
297	NE	ARG	A	849	-6.239	50.366	34.433	1.00	54.74
298	CZ	ARG	A	849	-5.141	51.111	34.334	1.00	54.79
299	NH1	ARG	A	849	-4.564	51.585	35.429	1.00	55.17
300	NH2	ARG	A	849	-4.617	51.376	33.146	1.00	54.99
301	N	MET	A	850	-4.562	45.458	34.21	1.00	47.8
302	CA	MET	A	850	-3.819	44.425	34.926	1.00	45.27
303	C	MET	A	850	-2.584	44.945	35.655	1.00	43.45
304	O	MET	A	850	-2.017	45.975	35.293	1.00	42.56
305	CB	MET	A	850	-3.374	43.34	33.951	1.00	45.5
306	CG	MET	A	850	-2.412	43.855	32.9	1.00	45.95
307	SD	MET	A	850	-1.625	42.55	31.956	1.00	47.19
308	CE	MET	A	850	-2.776	42.384	30.599	1.00	47.2
309	N	ASP	A	851	-2.171	44.212	36.683	1.00	41.28
310	CA	ASP	A	851	-0.987	44.571	37.449	1.00	39.27
311	C	ASP	A	851	0.241	44.296	36.598	1.00	37.06
312	O	ASP	A	851	0.203	43.488	35.666	1.00	36.58
313	CB	ASP	A	851	-0.896	43.74	38.735	1.00	40.25
314	CG	ASP	A	851	-1.864	44.203	39.805	1.00	41.24
315	OD1	ASP	A	851	-1.995	43.501	40.83	1.00	42.75
316	OD2	ASP	A	851	-2.488	45.268	39.632	1.00	41.66
317	N	ALA	A	852	1.333	44.97	36.93	1.00	34.59
318	CA	ALA	A	852	2.584	44.799	36.214	1.00	32.72
319	C	ALA	A	852	3.67	45.575	36.931	1.00	31.23

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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

320	O	ALA	A	852	3.394	46.345	37.846	1.00	30.91
321	CB	ALA	A	852	2.444	45.302	34.775	1.00	32.55
322	N	ALA	A	853	4.911	45.346	36.526	1.00	29.42
323	CA	ALA	A	853	6.038	46.054	37.1	1.00	28.63
324	C	ALA	A	853	6.677	46.707	35.899	1.00	28.61
325	O	ALA	A	853	6.554	46.205	34.783	1.00	27.57
326	CB	ALA	A	853	7.015	45.084	37.755	1.00	28.04
327	N	ILE	A	854	7.355	47.824	36.111	1.00	28.84
328	CA	ILE	A	854	7.977	48.492	34.99	1.00	29.81
329	C	ILE	A	854	9.44	48.814	35.211	1.00	30.57
330	O	ILE	A	854	9.814	49.481	36.174	1.00	29.86
331	CB	ILE	A	854	7.197	49.768	34.617	1.00	29.98
332	CG1	ILE	A	854	5.778	49.372	34.21	1.00	30.23
333	CG2	ILE	A	854	7.894	50.504	33.469	1.00	29.67
334	CD1	ILE	A	854	4.94	50.497	33.721	1.00	32.27
335	N	LYS	A	855	10.258	48.292	34.302	1.00	32.34
336	CA	LYS	A	855	11.698	48.494	34.306	1.00	34.61
337	C	LYS	A	855	11.98	49.702	33.415	1.00	36.33
338	O	LYS	A	855	11.692	49.684	32.217	1.00	35.66
339	CB	LYS	A	855	12.394	47.248	33.749	1.00	34.11
340	CG	LYS	A	855	13.892	47.393	33.522	1.00	34.2
341	CD	LYS	A	855	14.636	47.626	34.818	1.00	34.08
342	CE	LYS	A	855	16.142	47.644	34.593	1.00	34.27
343	NZ	LYS	A	855	16.872	47.924	35.865	1.00	33.94
344	N	ARG	A	856	12.528	50.752	34.015	1.00	38.9
345	CA	ARG	A	856	12.849	51.979	33.299	1.00	41.78
346	C	ARG	A	856	14.273	51.874	32.764	1.00	43.38
347	O	ARG	A	856	15.216	51.692	33.531	1.00	43.94
348	CB	ARG	A	856	12.713	53.17	34.254	1.00	42.47
349	CG	ARG	A	856	12.73	54.547	33.606	1.00	43.45
350	CD	ARG	A	856	12.181	55.588	34.583	1.00	44.24
351	NE	ARG	A	856	12.153	56.938	34.024	1.00	45.19
352	CZ	ARG	A	856	13.152	57.811	34.115	1.00	45.02
353	NH1	ARG	A	856	14.27	57.482	34.753	1.00	44.96
354	NH2	ARG	A	856	13.035	59.013	33.565	1.00	44.77
355	N	MET	A	857	14.422	51.974	31.447	1.00	45.01
356	CA	MET	A	857	15.733	51.877	30.814	1.00	46.68
357	C	MET	A	857	16.05	53.119	29.985	1.00	48.29
358	O	MET	A	857	15.271	53.517	29.117	1.00	48.15
359	CB	MET	A	857	15.791	50.637	29.918	1.00	46.23



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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

360	CG	MET	A	857	15.686	49.314	30.664	1.00	46.39
361	SD	MET	A	857	15.361	47.921	29.552	1.00	45.88
362	CE	MET	A	857	17.017	47.483	29.031	1.00	45.88
363	N	ALA	A	858	17.198	53.728	30.26	1.00	50.49
364	CA	ALA	A	858	17.629	54.92	29.538	1.00	52.93
365	C	ALA	A	858	18.196	54.525	28.182	1.00	54.6
366	O	ALA	A	858	19.08	53.671	28.095	1.00	54.83
367	CB	ALA	A	858	18.682	55.67	30.342	1.00	52.68
368	N	GLU	A	859	17.68	55.148	27.127	1.00	56.59
369	CA	GLU	A	859	18.136	54.864	25.771	1.00	58.81
370	C	GLU	A	859	19.424	55.611	25.436	1.00	59.91
371	O	GLU	A	859	19.548	56.22	24.373	1.00	60.25
372	CB	GLU	A	859	17.039	55.229	24.772	1.00	59.13
373	CG	GLU	A	859	16.014	54.135	24.592	1.00	60.11
374	CD	GLU	A	859	14.703	54.646	24.052	1.00	61.01
375	OE1	GLU	A	859	13.892	53.815	23.592	1.00	61.2
376	OE2	GLU	A	859	14.477	55.875	24.101	1.00	61.59
377	N	ALA	A	860	20.385	55.549	26.354	1.00	61.18
378	CA	ALA	A	860	21.67	56.213	26.179	1.00	62.12
379	CB	ALA	A	860	21.528	57.705	26.457	1.00	62.19
380	C	ALA	A	860	22.71	55.602	27.113	1.00	62.67
381	OT1	ALA	A	860	22.385	54.588	27.773	1.00	62.87
382	OT2	ALA	A	860	23.838	56.144	27.169	1.00	63.09
383	N	ALA	A	867	24.9	49.412	20.632	1.00	75.37
384	CA	ALA	A	867	25.35	49.829	21.991	1.00	75.34
385	C	ALA	A	867	24.957	48.796	23.047	1.00	75.37
386	O	ALA	A	867	24.409	47.736	22.729	1.00	75.47
387	CB	ALA	A	867	24.751	51.187	22.34	1.00	75.31
388	N	ASP	A	868	25.242	49.116	24.305	1.00	75.09
389	CA	ASP	A	868	24.929	48.232	25.422	1.00	74.54
390	C	ASP	A	868	23.415	48.025	25.521	1.00	73.75
391	O	ASP	A	868	22.933	46.893	25.574	1.00	73.79
392	CB	ASP	A	868	25.469	48.84	26.724	1.00	75.31
393	CG	ASP	A	868	25.498	47.846	27.874	1.00	76.1
394	OD1	ASP	A	868	24.42	47.345	28.263	1.00	76.74
395	OD2	ASP	A	868	26.603	47.569	28.392	1.00	76.36
396	N	PHE	A	869	22.675	49.131	25.534	1.00	72.51
397	CA	PHE	A	869	21.217	49.112	25.627	1.00	71.03
398	C	PHE	A	869	20.567	48.136	24.644	1.00	70.03
399	O	PHE	A	869	19.738	47.31	25.032	1.00	69.87

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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

400	CB	PHE	A	869	20.672	50.524	25.383	1.00	70.96
401	CG	PHE	A	869	19.172	50.598	25.309	1.00	70.66
402	CD1	PHE	A	869	18.393	50.376	26.438	1.00	70.43
403	CD2	PHE	A	869	18.539	50.885	24.104	1.00	70.55
404	CE1	PHE	A	869	17.004	50.438	26.368	1.00	70.34
405	CE2	PHE	A	869	17.152	50.949	24.023	1.00	70.39
406	CZ	PHE	A	869	16.383	50.726	25.158	1.00	70.24
407	N	ALA	A	870	20.945	48.241	23.374	1.00	68.68
408	CA	ALA	A	870	20.396	47.382	22.329	1.00	67.31
409	C	ALA	A	870	20.787	45.921	22.517	1.00	66.14
410	O	ALA	A	870	20.107	45.019	22.022	1.00	65.85
411	CB	ALA	A	870	20.859	47.873	20.96	1.00	67.34
412	N	GLY	A	871	21.885	45.694	23.233	1.00	64.86
413	CA	GLY	A	871	22.36	44.341	23.465	1.00	63.19
414	C	GLY	A	871	21.463	43.498	24.351	1.00	62.05
415	O	GLY	A	871	21.024	42.415	23.955	1.00	61.81
416	N	GLU	A	872	21.191	43.985	25.556	1.00	60.69
417	CA	GLU	A	872	20.343	43.256	26.488	1.00	59.54
418	C	GLU	A	872	18.899	43.266	26.004	1.00	58.23
419	O	GLU	A	872	18.145	42.321	26.243	1.00	57.9
420	CB	GLU	A	872	20.446	43.88	27.881	1.00	59.98
421	CG	GLU	A	872	19.997	45.324	27.951	1.00	60.9
422	CD	GLU	A	872	20.567	46.044	29.157	1.00	61.54
423	OE1	GLU	A	872	20.583	45.447	30.254	1.00	61.85
424	OE2	GLU	A	872	20.994	47.209	29.011	1.00	62.33
425	N	LEU	A	873	18.529	44.336	25.309	1.00	56.78
426	CA	LEU	A	873	17.182	44.484	24.779	1.00	55.14
427	C	LEU	A	873	16.942	43.426	23.713	1.00	53.83
428	O	LEU	A	873	15.82	42.959	23.517	1.00	53.65
429	CB	LEU	A	873	17.014	45.875	24.174	1.00	55.58
430	CG	LEU	A	873	15.589	46.287	23.819	1.00	55.8
431	CD1	LEU	A	873	14.753	46.34	25.089	1.00	56.01
432	CD2	LEU	A	873	15.603	47.643	23.129	1.00	55.92
433	N	GLU	A	874	18.013	43.054	23.025	1.00	52.42
434	CA	GLU	A	874	17.94	42.047	21.98	1.00	50.7
435	C	GLU	A	874	17.779	40.666	22.611	1.00	49
436	O	GLU	A	874	17.097	39.801	22.061	1.00	48.59
437	CB	GLU	A	874	19.203	42.099	21.119	1.00	51.88
438	CG	GLU	A	874	19.218	41.093	19.979	1.00	53.58
439	CD	GLU	A	874	20.352	41.333	19.001	1.00	54.42

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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

440	OE1	GLU	A	874	21.516	41.426	19.445	1.00	55.03
441	OE2	GLU	A	874	20.078	41.428	17.784	1.00	55.03
442	N	VAL	A	875	18.408	40.466	23.766	1.00	46.67
443	CA	VAL	A	875	18.308	39.195	24.477	1.00	44.49
444	C	VAL	A	875	16.907	39.047	25.076	1.00	43.2
445	O	VAL	A	875	16.344	37.954	25.103	1.00	42.33
446	CB	VAL	A	875	19.356	39.102	25.609	1.00	44.16
447	CG1	VAL	A	875	19.125	37.85	26.442	1.00	43.29
448	CG2	VAL	A	875	20.754	39.081	25.011	1.00	43.64
449	N	LEU	A	876	16.344	40.152	25.548	1.00	42.23
450	CA	LEU	A	876	15.009	40.122	26.136	1.00	41.58
451	C	LEU	A	876	13.953	39.698	25.112	1.00	41.27
452	O	LEU	A	876	12.961	39.063	25.461	1.00	40.8
453	CB	LEU	A	876	14.664	41.494	26.72	1.00	40.87
454	CG	LEU	A	876	15.406	41.87	28.008	1.00	40.58
455	CD1	LEU	A	876	15.135	43.33	28.351	1.00	40.2
456	CD2	LEU	A	876	14.961	40.955	29.151	1.00	39.63
457	N	CYS	A	877	14.179	40.039	23.847	1.00	41.25
458	CA	CYS	A	877	13.246	39.685	22.781	1.00	41.22
459	C	CYS	A	877	13.237	38.181	22.528	1.00	40.57
460	O	CYS	A	877	12.261	37.633	22.017	1.00	40.43
461	CB	CYS	A	877	13.622	40.417	21.488	1.00	42.55
462	SG	CYS	A	877	13.5	42.228	21.577	1.00	45.76
463	N	LYS	A	878	14.329	37.521	22.899	1.00	39.71
464	CA	LYS	A	878	14.476	36.082	22.711	1.00	39.12
465	C	LYS	A	878	13.779	35.225	23.758	1.00	38.18
466	O	LYS	A	878	13.572	34.035	23.547	1.00	38
467	CB	LYS	A	878	15.961	35.714	22.698	1.00	40.11
468	CG	LYS	A	878	16.725	36.273	21.531	1.00	41.15
469	CD	LYS	A	878	16.063	35.841	20.251	1.00	42.52
470	CE	LYS	A	878	16.866	36.258	19.049	1.00	43.43
471	NZ	LYS	A	878	16.099	35.933	17.829	1.00	44.72
472	N	LEU	A	879	13.424	35.83	24.885	1.00	37.55
473	CA	LEU	A	879	12.785	35.106	25.98	1.00	36.64
474	C	LEU	A	879	11.51	34.342	25.648	1.00	35.98
475	O	LEU	A	879	11.369	33.173	26.013	1.00	35.83
476	CB	LEU	A	879	12.499	36.065	27.138	1.00	36.2
477	CG	LEU	A	879	13.703	36.589	27.922	1.00	36.09
478	CD1	LEU	A	879	13.232	37.594	28.963	1.00	36.1
479	CD2	LEU	A	879	14.422	35.43	28.597	1.00	35.6

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TABLE 5  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

480	N	GLY	A	880	10.58	34.995	24.96	1.00	35.08
481	CA	GLY	A	880	9.323	34.338	24.654	1.00	34.13
482	C	GLY	A	880	8.49	34.313	25.926	1.00	33.52
483	O	GLY	A	880	8.639	35.191	26.776	1.00	33.87
484	N	HIS	A	881	7.624	33.316	26.077	1.00	32.85
485	CA	HIS	A	881	6.788	33.22	27.273	1.00	31.85
486	C	HIS	A	881	6.792	31.834	27.885	1.00	30.16
487	O	HIS	A	881	6.915	30.829	27.19	1.00	29.43
488	CB	HIS	A	881	5.346	33.626	26.959	1.00	34.13
489	CG	HIS	A	881	5.202	35.064	26.582	1.00	37.25
490	ND1	HIS	A	881	5.629	36.089	27.398	1.00	38.35
491	CD2	HIS	A	881	4.718	35.65	25.462	1.00	38.79
492	CE1	HIS	A	881	5.418	37.246	26.796	1.00	38.97
493	NE2	HIS	A	881	4.867	37.008	25.619	1.00	40.02
494	N	HIS	A	882	6.651	31.797	29.202	1.00	28.34
495	CA	HIS	A	882	6.63	30.546	29.939	1.00	26.59
496	C	HIS	A	882	6.099	30.849	31.338	1.00	25.24
497	O	HIS	A	882	6.39	31.9	31.909	1.00	24.1
498	CB	HIS	A	882	8.039	29.949	30.004	1.00	26.29
499	CG	HIS	A	882	8.07	28.545	30.516	1.00	26.5
500	ND1	HIS	A	882	7.972	28.24	31.857	1.00	26.46
501	CD2	HIS	A	882	8.113	27.359	29.861	1.00	26.27
502	CE1	HIS	A	882	7.949	26.926	32.004	1.00	26.89
503	NE2	HIS	A	882	8.032	26.369	30.808	1.00	26.1
504	N	PRO	A	883	5.287	29.944	31.895	1.00	24.17
505	CA	PRO	A	883	4.729	30.157	33.232	1.00	23.22
506	C	PRO	A	883	5.785	30.301	34.323	1.00	22.09
507	O	PRO	A	883	5.525	30.909	35.357	1.00	21.81
508	CB	PRO	A	883	3.869	28.915	33.451	1.00	23.13
509	CG	PRO	A	883	3.47	28.526	32.076	1.00	25.27
510	CD	PRO	A	883	4.732	28.725	31.283	1.00	24.1
511	N	ASN	A	884	6.976	29.755	34.093	1.00	20.78
512	CA	ASN	A	884	8.013	29.807	35.114	1.00	20.12
513	C	ASN	A	884	9.168	30.786	34.917	1.00	19.39
514	O	ASN	A	884	10.237	30.629	35.502	1.00	18.62
515	CB	ASN	A	884	8.52	28.387	35.368	1.00	18.93
516	CG	ASN	A	884	7.4	27.458	35.822	1.00	20.31
517	OD1	ASN	A	884	7.167	26.4	35.231	1.00	20.71
518	ND2	ASN	A	884	6.689	27.863	36.869	1.00	19.15
519	N	ILE	A	885	8.951	31.793	34.079	1.00	19.51

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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

520	CA	ILE	A	885	9.941	32.847	33.879	1.00	20.21
521	C	ILE	A	885	9.141	34.138	33.978	1.00	19.99
522	O	ILE	A	885	7.914	34.112	33.879	1.00	20.55
523	CB	ILE	A	885	10.615	32.829	32.474	1.00	19.97
524	CG1	ILE	A	885	9.593	33.197	31.395	1.00	20.96
525	CG2	ILE	A	885	11.256	31.484	32.213	1.00	19.49
526	CD1	ILE	A	885	10.214	33.483	30.016	1.00	21.59
527	N	ILE	A	886	9.818	35.257	34.194	1.00	20.11
528	CA	ILE	A	886	9.114	36.532	34.24	1.00	20.49
529	C	ILE	A	886	8.864	36.876	32.771	1.00	21.11
530	O	ILE	A	886	9.803	36.935	31.973	1.00	20.74
531	CB	ILE	A	886	9.971	37.643	34.879	1.00	20.64
532	CG1	ILE	A	886	10.134	37.387	36.384	1.00	20.81
533	CG2	ILE	A	886	9.337	38.999	34.611	1.00	19.69
534	CD1	ILE	A	886	8.85	37.545	37.195	1.00	20.87
535	N	ASN	A	887	7.6	37.068	32.413	1.00	21.74
536	CA	ASN	A	887	7.238	37.394	31.041	1.00	23.6
537	C	ASN	A	887	7.208	38.896	30.82	1.00	23.93
538	O	ASN	A	887	6.921	39.652	31.739	1.00	23.11
539	CB	ASN	A	887	5.855	36.824	30.703	1.00	24.65
540	CG	ASN	A	887	5.841	35.308	30.644	1.00	26.68
541	OD1	ASN	A	887	6.673	34.69	29.978	1.00	26.03
542	ND2	ASN	A	887	4.879	34.702	31.328	1.00	28.12
543	N	LEU	A	888	7.517	39.317	29.597	1.00	26.03
544	CA	LEU	A	888	7.481	40.729	29.228	1.00	28.08
545	C	LEU	A	888	6.077	40.975	28.684	1.00	29
546	O	LEU	A	888	5.581	40.213	27.854	1.00	29.37
547	CB	LEU	A	888	8.52	41.036	28.146	1.00	28.9
548	CG	LEU	A	888	9.966	40.634	28.453	1.00	30.62
549	CD1	LEU	A	888	10.87	41.105	27.313	1.00	31.98
550	CD2	LEU	A	888	10.419	41.24	29.772	1.00	31.28
551	N	LEU	A	889	5.432	42.034	29.154	1.00	30.57
552	CA	LEU	A	889	4.075	42.342	28.725	1.00	31.68
553	C	LEU	A	889	4.027	43.37	27.601	1.00	32.96
554	O	LEU	A	889	2.973	43.605	27.009	1.00	33.39
555	CB	LEU	A	889	3.274	42.846	29.919	1.00	31.11
556	CG	LEU	A	889	3.404	41.969	31.165	1.00	31.57
557	CD1	LEU	A	889	2.659	42.605	32.327	1.00	30.88
558	CD2	LEU	A	889	2.865	40.584	30.868	1.00	31.4
559	N	GLY	A	890	5.175	43.968	27.303	1.00	34.07

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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

560	CA	GLY	A	890	5.243	44.977	26.261	1.00	35.62
561	C	GLY	A	890	6.084	46.14	26.748	1.00	36.68
562	O	GLY	A	890	6.587	46.107	27.87	1.00	36.77
563	N	ALA	A	891	6.244	47.167	25.922	1.00	37.61
564	CA	ALA	A	891	7.042	48.321	26.32	1.00	38.76
565	C	ALA	A	891	6.562	49.628	25.694	1.00	39.81
566	O	ALA	A	891	5.831	49.635	24.699	1.00	39.79
567	CB	ALA	A	891	8.506	48.082	25.977	1.00	38.22
568	N	CYS	A	892	6.993	50.734	26.289	1.00	40.79
569	CA	CYS	A	892	6.62	52.065	25.833	1.00	42.07
570	C	CYS	A	892	7.797	53.022	25.95	1.00	42.53
571	O	CYS	A	892	8.378	53.176	27.027	1.00	42.35
572	CB	CYS	A	892	5.456	52.595	26.673	1.00	42.43
573	SG	CYS	A	892	5.183	54.38	26.535	1.00	43.92
574	N	GLU	A	893	8.155	53.664	24.844	1.00	43.17
575	CA	GLU	A	893	9.256	54.618	24.873	1.00	43.99
576	C	GLU	A	893	8.668	55.978	25.225	1.00	42.93
577	O	GLU	A	893	7.68	56.41	24.63	1.00	42.5
578	CB	GLU	A	893	9.958	54.676	23.521	1.00	45.8
579	CG	GLU	A	893	11.368	55.222	23.611	1.00	49.17
580	CD	GLU	A	893	12.064	55.258	22.267	1.00	51.53
581	OE1	GLU	A	893	12.026	54.233	21.549	1.00	52.95
582	OE2	GLU	A	893	12.657	56.307	21.933	1.00	53.05
583	N	HIS	A	894	9.274	56.653	26.193	1.00	42.38
584	CA	HIS	A	894	8.759	57.939	26.632	1.00	41.87
585	C	HIS	A	894	9.853	58.874	27.126	1.00	41.21
586	O	HIS	A	894	10.604	58.544	28.045	1.00	40.8
587	CB	HIS	A	894	7.74	57.718	27.752	1.00	42.15
588	CG	HIS	A	894	6.987	58.95	28.146	1.00	42.76
589	ND1	HIS	A	894	5.986	59.49	27.369	1.00	42.91
590	CD2	HIS	A	894	7.073	59.732	29.248	1.00	42.78
591	CE1	HIS	A	894	5.483	60.551	27.978	1.00	42.96
592	NE2	HIS	A	894	6.126	60.719	29.119	1.00	43.21
593	N	ARG	A	895	9.921	60.048	26.509	1.00	40.32
594	CA	ARG	A	895	10.892	61.07	26.865	1.00	39.33
595	C	ARG	A	895	12.299	60.542	27.13	1.00	39.43
596	O	ARG	A	895	12.846	60.707	28.222	1.00	38.88
597	CB	ARG	A	895	10.373	61.869	28.067	1.00	38.53
598	CG	ARG	A	895	9.038	62.539	27.776	1.00	37.75
599	CD	ARG	A	895	8.513	63.398	28.916	1.00	37.39

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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

600	NE	ARG	A	895	7.184	63.916	28.591	1.00	37.52
601	CZ	ARG	A	895	6.458	64.707	29.378	1.00	37.96
602	NH1	ARG	A	895	6.922	65.092	30.558	1.00	38.38
603	NH2	ARG	A	895	5.252	65.102	28.989	1.00	37.96
604	N	GLY	A	896	12.872	59.905	26.11	1.00	39.63
605	CA	GLY	A	896	14.226	59.381	26.198	1.00	39.77
606	C	GLY	A	896	14.441	58.159	27.067	1.00	39.89
607	O	GLY	A	896	15.575	57.866	27.452	1.00	40.25
608	N	PHE	A	897	13.369	57.434	27.368	1.00	39.56
609	CA	PHE	A	897	13.471	56.246	28.211	1.00	38.44
610	C	PHE	A	897	12.572	55.119	27.749	1.00	37.83
611	O	PHE	A	897	11.444	55.348	27.315	1.00	37.87
612	CB	PHE	A	897	13.099	56.596	29.65	1.00	38.49
613	CG	PHE	A	897	14.182	57.295	30.403	1.00	38.86
614	CD1	PHE	A	897	15.174	56.567	31.05	1.00	38.8
615	CD2	PHE	A	897	14.214	58.683	30.471	1.00	38.93
616	CE1	PHE	A	897	16.182	57.209	31.756	1.00	39.25
617	CE2	PHE	A	897	15.22	59.338	31.175	1.00	39.27
618	CZ	PHE	A	897	16.206	58.6	31.82	1.00	39.44
619	N	LEU	A	898	13.07	53.894	27.846	1.00	37.34
620	CA	LEU	A	898	12.265	52.745	27.473	1.00	36.87
621	C	LEU	A	898	11.616	52.236	28.75	1.00	35.95
622	O	LEU	A	898	12.296	51.989	29.742	1.00	35.89
623	CB	LEU	A	898	13.128	51.643	26.857	1.00	37.46
624	CG	LEU	A	898	12.355	50.36	26.525	1.00	37.9
625	CD1	LEU	A	898	11.236	50.657	25.54	1.00	37.47
626	CD2	LEU	A	898	13.308	49.332	25.953	1.00	38.5
627	N	TYR	A	899	10.297	52.104	28.733	1.00	35.5
628	CA	TYR	A	899	9.568	51.616	29.896	1.00	34.77
629	C	TYR	A	899	9.078	50.205	29.616	1.00	34.02
630	O	TYR	A	899	8.043	50.006	28.981	1.00	33.82
631	CB	TYR	A	899	8.402	52.546	30.197	1.00	35.39
632	CG	TYR	A	899	8.842	53.861	30.799	1.00	37.41
633	CD1	TYR	A	899	8.98	54.004	32.178	1.00	37.45
634	CD2	TYR	A	899	9.133	54.963	29.988	1.00	37.76
635	CE1	TYR	A	899	9.391	55.206	32.737	1.00	38.53
636	CE2	TYR	A	899	9.55	56.17	30.54	1.00	38.14
637	CZ	TYR	A	899	9.675	56.284	31.915	1.00	38.82
638	OH	TYR	A	899	10.086	57.472	32.475	1.00	39.7
639	N	LEU	A	900	9.836	49.228	30.1	1.00	32.56

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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

640	CA	LEU	A	900	9.517	47.823	29.877	1.00	31.66
641	C	LEU	A	900	8.554	47.241	30.906	1.00	30.53
642	O	LEU	A	900	8.839	47.16	32.096	1.00	30.86
643	CB	LEU	A	900	10.814	47.013	29.856	1.00	32
644	CG	LEU	A	900	10.739	45.514	29.571	1.00	32.16
645	CD1	LEU	A	900	10.118	45.258	28.2	1.00	32.11
646	CD2	LEU	A	900	12.149	44.941	29.634	1.00	32.1
647	N	ALA	A	901	7.374	46.839	30.445	1.00	28.73
648	CA	ALA	A	901	6.38	46.253	31.333	1.00	27.74
649	C	ALA	A	901	6.672	44.766	31.473	1.00	26.95
650	O	ALA	A	901	6.829	44.06	30.474	1.00	26.8
651	CB	ALA	A	901	4.979	46.462	30.769	1.00	27.34
652	N	ILE	A	902	6.759	44.299	32.713	1.00	26.28
653	CA	ILE	A	902	7.032	42.89	32.977	1.00	25.36
654	C	ILE	A	902	6.054	42.36	34.011	1.00	25.12
655	O	ILE	A	902	5.438	43.124	34.75	1.00	25.11
656	CB	ILE	A	902	8.471	42.67	33.508	1.00	24.4
657	CG1	ILE	A	902	8.646	43.366	34.858	1.00	24.03
658	CG2	ILE	A	902	9.485	43.208	32.511	1.00	24.93
659	CD1	ILE	A	902	10.013	43.168	35.482	1.00	22.88
660	N	GLU	A	903	5.926	41.041	34.058	1.00	24.93
661	CA	GLU	A	903	5.028	40.375	34.987	1.00	24.9
662	C	GLU	A	903	5.285	40.824	36.419	1.00	24.87
663	O	GLU	A	903	6.439	40.966	36.838	1.00	24.67
664	CB	GLU	A	903	5.234	38.869	34.891	1.00	25.9
665	CG	GLU	A	903	3.972	38.049	34.944	1.00	27.81
666	CD	GLU	A	903	4.259	36.575	34.771	1.00	27.87
667	OE1	GLU	A	903	5.101	36.244	33.91	1.00	27.41
668	OE2	GLU	A	903	3.645	35.756	35.489	1.00	28.56
669	N	TYR	A	904	4.206	41.04	37.165	1.00	23.85
670	CA	TYR	A	904	4.291	41.454	38.557	1.00	23.56
671	C	TYR	A	904	4.224	40.228	39.46	1.00	23.93
672	O	TYR	A	904	3.41	39.334	39.234	1.00	24.84
673	CB	TYR	A	904	3.134	42.391	38.894	1.00	22.85
674	CG	TYR	A	904	2.946	42.647	40.371	1.00	22.68
675	CD1	TYR	A	904	3.942	43.26	41.13	1.00	22.71
676	CD2	TYR	A	904	1.762	42.287	41.01	1.00	23.14
677	CE1	TYR	A	904	3.763	43.513	42.489	1.00	22.98
678	CE2	TYR	A	904	1.572	42.533	42.365	1.00	23.22
679	CZ	TYR	A	904	2.574	43.147	43.097	1.00	23.59



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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

680	OH	TYR	A	904	2.376	43.398	44.438	1.00	24.17
681	N	ALA	A	905	5.074	40.199	40.482	1.00	23.71
682	CA	ALA	A	905	5.116	39.097	41.439	1.00	24.06
683	C	ALA	A	905	4.594	39.59	42.785	1.00	23.49
684	O	ALA	A	905	5.287	40.296	43.51	1.00	23.76
685	CB	ALA	A	905	6.544	38.585	41.587	1.00	23.85
686	N	PRO	A	906	3.359	39.212	43.134	1.00	23.96
687	CA	PRO	A	906	2.683	39.589	44.381	1.00	23.56
688	C	PRO	A	906	3.401	39.223	45.679	1.00	23.64
689	O	PRO	A	906	3.328	39.961	46.659	1.00	23.19
690	CB	PRO	A	906	1.332	38.871	44.279	1.00	23.68
691	CG	PRO	A	906	1.11	38.75	42.806	1.00	24.49
692	CD	PRO	A	906	2.482	38.369	42.301	1.00	24.13
693	N	HIS	A	907	4.108	38.1	45.69	1.00	23.41
694	CA	HIS	A	907	4.755	37.663	46.921	1.00	22.97
695	C	HIS	A	907	6.271	37.814	47.059	1.00	22.71
696	O	HIS	A	907	6.896	37.093	47.829	1.00	22.55
697	CB	HIS	A	907	4.332	36.218	47.193	1.00	23.67
698	CG	HIS	A	907	2.863	35.988	47.006	1.00	23.96
699	ND1	HIS	A	907	1.914	36.488	47.874	1.00	24.53
700	CD2	HIS	A	907	2.177	35.375	46.011	1.00	23.91
701	CE1	HIS	A	907	0.708	36.195	47.419	1.00	24.06
702	NE2	HIS	A	907	0.841	35.521	46.29	1.00	24.69
703	N	GLY	A	908	6.857	38.753	46.324	1.00	22.79
704	CA	GLY	A	908	8.289	38.99	46.429	1.00	21.49
705	C	GLY	A	908	9.199	37.879	45.942	1.00	20.63
706	O	GLY	A	908	8.759	36.962	45.246	1.00	19.73
707	N	ASN	A	909	10.475	37.96	46.314	1.00	19.89
708	CA	ASN	A	909	11.452	36.961	45.894	1.00	20.39
709	C	ASN	A	909	11.413	35.738	46.799	1.00	19.43
710	O	ASN	A	909	11.143	35.837	47.996	1.00	19.98
711	CB	ASN	A	909	12.864	37.571	45.852	1.00	21.16
712	CG	ASN	A	909	13.44	37.827	47.231	1.00	22.89
713	OD1	ASN	A	909	13.763	36.893	47.968	1.00	23.48
714	ND2	ASN	A	909	13.572	39.1	47.587	1.00	23.13
715	N	LEU	A	910	11.683	34.581	46.212	1.00	19.13
716	CA	LEU	A	910	11.64	33.316	46.932	1.00	18.54
717	C	LEU	A	910	12.479	33.271	48.205	1.00	19.02
718	O	LEU	A	910	12.064	32.686	49.198	1.00	19.4
719	CB	LEU	A	910	12.058	32.184	45.994	1.00	17.39

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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

720	CG	LEU	A	910	12.011	30.754	46.538	1.00	17.49
721	CD1	LEU	A	910	10.608	30.404	47.014	1.00	16.17
722	CD2	LEU	A	910	12.429	29.807	45.431	1.00	16.87
723	N	LEU	A	911	13.663	33.872	48.18	1.00	19.57
724	CA	LEU	A	911	14.516	33.858	49.36	1.00	19.95
725	C	LEU	A	911	13.787	34.424	50.582	1.00	20.28
726	O	LEU	A	911	13.708	33.772	51.62	1.00	20.89
727	CB	LEU	A	911	15.81	34.647	49.098	1.00	19.78
728	CG	LEU	A	911	16.764	34.771	50.29	1.00	20.41
729	CD1	LEU	A	911	17.045	33.39	50.885	1.00	19.74
730	CD2	LEU	A	911	18.059	35.449	49.838	1.00	20.39
731	N	ASP	A	912	13.253	35.634	50.464	1.00	20.79
732	CA	ASP	A	912	12.541	36.244	51.578	1.00	21.69
733	C	ASP	A	912	11.278	35.478	51.941	1.00	20.65
734	O	ASP	A	912	10.915	35.393	53.112	1.00	20.32
735	CB	ASP	A	912	12.154	37.692	51.261	1.00	23.57
736	CG	ASP	A	912	13.351	38.622	51.223	1.00	26.54
737	OD1	ASP	A	912	14.319	38.387	51.982	1.00	28.32
738	OD2	ASP	A	912	13.316	39.598	50.444	1.00	27.51
739	N	PHE	A	913	10.607	34.937	50.931	1.00	20.41
740	CA	PHE	A	913	9.375	34.196	51.15	1.00	20
741	C	PHE	A	913	9.645	32.963	52.001	1.00	19.85
742	O	PHE	A	913	8.848	32.612	52.872	1.00	19.61
743	CB	PHE	A	913	8.76	33.782	49.813	1.00	19.38
744	CG	PHE	A	913	7.368	33.222	49.935	1.00	19.74
745	CD1	PHE	A	913	6.291	34.054	50.229	1.00	19.6
746	CD2	PHE	A	913	7.135	31.865	49.758	1.00	19.66
747	CE1	PHE	A	913	4.999	33.543	50.342	1.00	19.53
748	CE2	PHE	A	913	5.848	31.336	49.867	1.00	19.54
749	CZ	PHE	A	913	4.776	32.18	50.161	1.00	20.36
750	N	LEU	A	914	10.773	32.31	51.742	1.00	19.17
751	CA	LEU	A	914	11.153	31.118	52.49	1.00	19.24
752	C	LEU	A	914	11.469	31.475	53.94	1.00	19.47
753	O	LEU	A	914	11.001	30.814	54.871	1.00	19.97
754	CB	LEU	A	914	12.378	30.462	51.848	1.00	18.62
755	CG	LEU	A	914	12.217	29.829	50.459	1.00	18.62
756	CD1	LEU	A	914	13.588	29.533	49.862	1.00	18.3
757	CD2	LEU	A	914	11.398	28.541	50.571	1.00	18.67
758	N	ARG	A	915	12.25	32.533	54.13	1.00	19.31
759	CA	ARG	A	915	12.635	32.957	55.467	1.00	19.18

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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

760	C	ARG	A	915	11.468	33.432	56.314	1.00	19.31
761	O	ARG	A	915	11.443	33.186	57.518	1.00	17.9
762	CB	ARG	A	915	13.703	34.052	55.388	1.00	19.16
763	CG	ARG	A	915	15.036	33.535	54.882	1.00	19.15
764	CD	ARG	A	915	16.056	34.64	54.679	1.00	19.59
765	NE	ARG	A	915	17.34	34.084	54.265	1.00	21.3
766	CZ	ARG	A	915	18.383	34.805	53.866	1.00	22.41
767	NH1	ARG	A	915	19.508	34.199	53.51	1.00	23.64
768	NH2	ARG	A	915	18.3	36.127	53.809	1.00	22.63
769	N	LYS	A	916	10.495	34.093	55.689	1.00	19.83
770	CA	LYS	A	916	9.344	34.592	56.425	1.00	20.99
771	C	LYS	A	916	8.379	33.483	56.84	1.00	20.9
772	O	LYS	A	916	7.445	33.722	57.611	1.00	20.71
773	CB	LYS	A	916	8.603	35.654	55.61	1.00	23.11
774	CG	LYS	A	916	9.394	36.948	55.395	1.00	25.94
775	CD	LYS	A	916	8.495	38.041	54.812	1.00	28.94
776	CE	LYS	A	916	9.292	39.244	54.323	1.00	30.74
777	NZ	LYS	A	916	10.14	39.822	55.406	1.00	33.02
778	N	SER	A	917	8.612	32.272	56.343	1.00	19.95
779	CA	SER	A	917	7.76	31.135	56.686	1.00	19.78
780	C	SER	A	917	8.263	30.388	57.923	1.00	19.55
781	O	SER	A	917	7.63	29.431	58.367	1.00	19.53
782	CB	SER	A	917	7.685	30.148	55.518	1.00	19.99
783	OG	SER	A	917	8.8	29.272	55.522	1.00	19.1
784	N	ARG	A	918	9.405	30.812	58.464	1.00	19.27
785	CA	ARG	A	918	9.984	30.17	59.648	1.00	18.81
786	C	ARG	A	918	9.192	30.566	60.901	1.00	19.63
787	O	ARG	A	918	9.665	31.348	61.732	1.00	18.49
788	CB	ARG	A	918	11.447	30.587	59.813	1.00	18.16
789	CG	ARG	A	918	12.345	30.215	58.647	1.00	17.53
790	CD	ARG	A	918	13.798	30.52	58.982	1.00	17.19
791	NE	ARG	A	918	14.717	29.896	58.043	1.00	17.15
792	CZ	ARG	A	918	16.022	29.76	58.256	1.00	18.33
793	NH1	ARG	A	918	16.79	29.175	57.346	1.00	19.06
794	NH2	ARG	A	918	16.564	30.203	59.381	1.00	17.42
795	N	VAL	A	919	7.997	29.997	61.035	1.00	20.08
796	CA	VAL	A	919	7.1	30.302	62.143	1.00	20.09
797	C	VAL	A	919	7.663	30.028	63.535	1.00	21.11
798	O	VAL	A	919	7.291	30.703	64.491	1.00	20.8
799	CB	VAL	A	919	5.727	29.577	61.948	1.00	20.98

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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

800	CG1	VAL	A	919	5.92	28.076	61.946	1.00	20.86
801	CG2	VAL	A	919	4.739	30.007	63.027	1.00	21.03
802	N	LEU	A	920	8.564	29.056	63.661	1.00	21.75
803	CA	LEU	A	920	9.153	28.766	64.96	1.00	22.53
804	C	LEU	A	920	9.936	29.981	65.469	1.00	23.15
805	O	LEU	A	920	10.024	30.211	66.678	1.00	22.77
806	CB	LEU	A	920	10.077	27.547	64.879	1.00	23.71
807	CG	LEU	A	920	10.752	27.149	66.2	1.00	23.84
808	CD1	LEU	A	920	9.702	26.731	67.22	1.00	24.31
809	CD2	LEU	A	920	11.721	26.007	65.947	1.00	25.23
810	N	GLU	A	921	10.494	30.764	64.548	1.00	23.64
811	CA	GLU	A	921	11.25	31.954	64.928	1.00	25.41
812	C	GLU	A	921	10.395	33.214	65.011	1.00	24.74
813	O	GLU	A	921	10.604	34.06	65.882	1.00	25.25
814	CB	GLU	A	921	12.414	32.185	63.961	1.00	27.63
815	CG	GLU	A	921	13.499	31.161	64.144	1.00	33.37
816	CD	GLU	A	921	14.789	31.502	63.44	1.00	36.17
817	OE1	GLU	A	921	14.775	31.638	62.195	1.00	37.62
818	OE2	GLU	A	921	15.82	31.625	64.142	1.00	37.03
819	N	THR	A	922	9.428	33.338	64.114	1.00	24.18
820	CA	THR	A	922	8.565	34.509	64.112	1.00	23.93
821	C	THR	A	922	7.524	34.458	65.23	1.00	23.77
822	O	THR	A	922	7.108	35.493	65.738	1.00	24.19
823	CB	THR	A	922	7.826	34.654	62.773	1.00	24.25
824	OG1	THR	A	922	7.012	33.494	62.551	1.00	24
825	CG2	THR	A	922	8.819	34.801	61.623	1.00	24.68
826	N	ASP	A	923	7.113	33.255	65.617	1.00	23.25
827	CA	ASP	A	923	6.096	33.095	66.659	1.00	23.01
828	C	ASP	A	923	6.157	31.678	67.211	1.00	21.89
829	O	ASP	A	923	5.303	30.85	66.914	1.00	20.44
830	CB	ASP	A	923	4.709	33.366	66.057	1.00	23.92
831	CG	ASP	A	923	3.599	33.419	67.102	1.00	24.55
832	OD1	ASP	A	923	3.867	33.232	68.307	1.00	26.04
833	OD2	ASP	A	923	2.443	33.654	66.705	1.00	23.86
834	N	PRO	A	924	7.181	31.383	68.026	1.00	21.97
835	CA	PRO	A	924	7.362	30.055	68.621	1.00	22.45
836	C	PRO	A	924	6.151	29.478	69.347	1.00	22.74
837	O	PRO	A	924	5.871	28.287	69.238	1.00	22.77
838	CB	PRO	A	924	8.571	30.247	69.548	1.00	23.11
839	CG	PRO	A	924	8.554	31.713	69.859	1.00	22.46

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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

840	CD	PRO	A	924	8.203	32.317	68.526	1.00	21.95
841	N	ALA	A	925	5.43	30.308	70.09	1.00	22.88
842	CA	ALA	A	925	4.262	29.808	70.803	1.00	23.14
843	C	ALA	A	925	3.296	29.182	69.798	1.00	22.89
844	O	ALA	A	925	2.752	28.102	70.028	1.00	23.08
845	CB	ALA	A	925	3.584	30.937	71.563	1.00	23.43
846	N	PHE	A	926	3.11	29.85	68.664	1.00	23.49
847	CA	PHE	A	926	2.208	29.344	67.631	1.00	22.16
848	C	PHE	A	926	2.762	28.091	66.971	1.00	22.59
849	O	PHE	A	926	2.022	27.142	66.704	1.00	22.74
850	CB	PHE	A	926	1.968	30.412	66.565	1.00	21.16
851	CG	PHE	A	926	0.98	29.995	65.514	1.00	21.77
852	CD1	PHE	A	926	1.352	29.119	64.496	1.00	20.95
853	CD2	PHE	A	926	-0.34	30.441	65.569	1.00	21.7
854	CE1	PHE	A	926	0.426	28.687	63.546	1.00	21.1
855	CE2	PHE	A	926	-1.28	30.015	64.621	1.00	21.96
856	CZ	PHE	A	926	-0.893	29.135	63.608	1.00	21.33
857	N	ALA	A	927	4.062	28.098	66.698	1.00	22.89
858	CA	ALA	A	927	4.717	26.963	66.059	1.00	23.26
859	C	ALA	A	927	4.577	25.719	66.926	1.00	24.13
860	O	ALA	A	927	4.3	24.624	66.421	1.00	23.88
861	CB	ALA	A	927	6.201	27.274	65.82	1.00	22.84
862	N	ILE	A	928	4.771	25.888	68.23	1.00	24.45
863	CA	ILE	A	928	4.659	24.768	69.161	1.00	26.24
864	C	ILE	A	928	3.226	24.253	69.211	1.00	26.73
865	O	ILE	A	928	2.971	23.059	69.018	1.00	26.88
866	CB	ILE	A	928	5.068	25.172	70.602	1.00	27.09
867	CG1	ILE	A	928	6.513	25.668	70.621	1.00	27.72
868	CG2	ILE	A	928	4.9	23.98	71.544	1.00	27.54
869	CD1	ILE	A	928	7.49	24.703	70.035	1.00	29.34
870	N	ALA	A	929	2.296	25.168	69.466	1.00	26.7
871	CA	ALA	A	929	0.878	24.836	69.562	1.00	27.25
872	C	ALA	A	929	0.327	24.111	68.337	1.00	27.02
873	O	ALA	A	929	-0.612	23.322	68.445	1.00	26.9
874	CB	ALA	A	929	0.089	26.112	69.811	1.00	26.93
875	N	ASN	A	930	0.922	24.363	67.175	1.00	27.22
876	CA	ASN	A	930	0.444	23.758	65.936	1.00	27.02
877	C	ASN	A	930	1.458	22.833	65.272	1.00	26.91
878	O	ASN	A	930	1.31	22.469	64.107	1.00	26.67
879	CB	ASN	A	930	0.024	24.872	64.978	1.00	26.86

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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

880	CG	ASN	A	930	-1.13	25.701	65.527	1.00	27.49
881	OD1	ASN	A	930	-2.266	25.233	65.586	1.00	28.15
882	ND2	ASN	A	930	-0.84	26.93	65.944	1.00	26.15
883	N	SER	A	931	2.485	22.462	66.032	1.00	26.99
884	CA	SER	A	931	3.541	21.568	65.563	1.00	26.94
885	C	SER	A	931	3.996	21.88	64.14	1.00	26.6
886	O	SER	A	931	4.044	21.003	63.28	1.00	26.16
887	CB	SER	A	931	3.054	20.123	65.667	1.00	27.5
888	OG	SER	A	931	2.739	19.82	67.022	1.00	28.02
889	N	THR	A	932	4.354	23.138	63.913	1.00	25.8
890	CA	THR	A	932	4.784	23.586	62.596	1.00	25.25
891	C	THR	A	932	6.096	24.374	62.642	1.00	24.16
892	O	THR	A	932	6.245	25.302	63.437	1.00	23.8
893	CB	THR	A	932	3.693	24.478	61.946	1.00	25.53
894	OG1	THR	A	932	4.171	24.997	60.701	1.00	27.23
895	CG2	THR	A	932	3.346	25.65	62.862	1.00	25.31
896	N	ALA	A	933	7.038	23.992	61.786	1.00	23.06
897	CA	ALA	A	933	8.324	24.677	61.697	1.00	22.34
898	C	ALA	A	933	8.296	25.654	60.511	1.00	21.89
899	O	ALA	A	933	9.154	26.520	60.388	1.00	21.49
900	CB	ALA	A	933	9.455	23.663	61.521	1.00	21.69
901	N	SER	A	934	7.305	25.498	59.637	1.00	21.28
902	CA	SER	A	934	7.166	26.376	58.482	1.00	21.08
903	C	SER	A	934	5.714	26.454	58.023	1.00	21.58
904	O	SER	A	934	4.995	25.461	58.059	1.00	21.87
905	CB	SER	A	934	8.046	25.881	57.326	1.00	20.56
906	OG	SER	A	934	7.88	26.688	56.168	1.00	18.6
907	N	THR	A	935	5.281	27.636	57.598	1.00	21.84
908	CA	THR	A	935	3.91	27.815	57.115	1.00	22.4
909	C	THR	A	935	3.695	27.088	55.782	1.00	22.71
910	O	THR	A	935	2.56	26.851	55.36	1.00	22.19
911	CB	THR	A	935	3.592	29.299	56.897	1.00	22.6
912	OG1	THR	A	935	4.535	29.849	55.972	1.00	23.34
913	CG2	THR	A	935	3.667	30.069	58.211	1.00	21.79
914	N	LEU	A	936	4.794	26.728	55.129	1.00	22.99
915	CA	LEU	A	936	4.745	26.05	53.84	1.00	23.37
916	C	LEU	A	936	4.806	24.539	53.993	1.00	24.14
917	O	LEU	A	936	5.351	24.024	54.968	1.00	25.53
918	CB	LEU	A	936	5.913	26.516	52.973	1.00	22.65
919	CG	LEU	A	936	6.031	28.036	52.837	1.00	22.95

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TABLE 5  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

920	CD1	LEU	A	936	7.319	28.405	52.12	1.00	22.09
921	CD2	LEU	A	936	4.81	28.564	52.105	1.00	22.4
922	N	SER	A	937	4.259	23.83	53.015	1.00	24.17
923	CA	SER	A	937	4.258	22.373	53.037	1.00	23.59
924	C	SER	A	937	5.38	21.824	52.17	1.00	23.28
925	O	SER	A	937	5.962	22.54	51.36	1.00	23.78
926	CB	SER	A	937	2.928	21.849	52.499	1.00	23.45
927	OG	SER	A	937	2.741	22.274	51.158	1.00	22.1
928	N	SER	A	938	5.655	20.537	52.335	1.00	22.96
929	CA	SER	A	938	6.677	19.848	51.559	1.00	23.25
930	C	SER	A	938	6.335	19.9	50.064	1.00	23.29
931	O	SER	A	938	7.207	20.14	49.224	1.00	22.8
932	CB	SER	A	938	6.782	18.389	52.022	1.00	23.03
933	OG	SER	A	938	7.685	17.655	51.213	1.00	24.53
934	N	GLN	A	939	5.065	19.674	49.732	1.00	23.8
935	CA	GLN	A	939	4.627	19.708	48.337	1.00	24.51
936	C	GLN	A	939	4.92	21.064	47.683	1.00	23.74
937	O	GLN	A	939	5.448	21.13	46.569	1.00	23.88
938	CB	GLN	A	939	3.127	19.42	48.236	1.00	26.49
939	CG	GLN	A	939	2.732	17.965	48.449	1.00	30.69
940	CD	GLN	A	939	3.38	17.017	47.444	1.00	32.5
941	OE1	GLN	A	939	4.37	16.353	47.748	1.00	33.33
942	NE2	GLN	A	939	2.822	16.958	46.241	1.00	33.32
943	N	GLN	A	940	4.57	22.142	48.378	1.00	22.76
944	CA	GLN	A	940	4.803	23.479	47.855	1.00	22.58
945	C	GLN	A	940	6.301	23.711	47.644	1.00	21.87
946	O	GLN	A	940	6.702	24.24	46.608	1.00	22.3
947	CB	GLN	A	940	4.219	24.54	48.804	1.00	23.22
948	CG	GLN	A	940	4.529	25.976	48.392	1.00	23.5
949	CD	GLN	A	940	3.904	26.352	47.062	1.00	24.6
950	OE1	GLN	A	940	2.883	27.03	47.019	1.00	26.55
951	NE2	GLN	A	940	4.514	25.909	45.969	1.00	24.77
952	N	LEU	A	941	7.128	23.305	48.606	1.00	20.72
953	CA	LEU	A	941	8.576	23.481	48.464	1.00	21.4
954	C	LEU	A	941	9.077	22.748	47.215	1.00	20.95
955	O	LEU	A	941	9.835	23.312	46.418	1.00	21.13
956	CB	LEU	A	941	9.31	22.972	49.707	1.00	20.6
957	CG	LEU	A	941	9	23.74	50.998	1.00	21.3
958	CD1	LEU	A	941	9.596	23.012	52.185	1.00	19.86
959	CD2	LEU	A	941	9.553	25.159	50.906	1.00	20.4

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TABLE 5  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

960	N	LEU	A	942	8.645	21.499	47.046	1.00	20.69
961	CA	LEU	A	942	9.025	20.713	45.879	1.00	20.38
962	C	LEU	A	942	8.452	21.332	44.609	1.00	20.08
963	O	LEU	A	942	9.069	21.254	43.552	1.00	20.9
964	CB	LEU	A	942	8.54	19.265	46.011	1.00	21.36
965	CG	LEU	A	942	9.31	18.361	46.976	1.00	22.69
966	CD1	LEU	A	942	8.848	16.92	46.806	1.00	23.37
967	CD2	LEU	A	942	10.808	18.466	46.696	1.00	23.21
968	N	HIS	A	943	7.27	21.935	44.697	1.00	19.88
969	CA	HIS	A	943	6.69	22.58	43.519	1.00	20.21
970	C	HIS	A	943	7.497	23.808	43.088	1.00	19.27
971	O	HIS	A	943	7.562	24.129	41.9	1.00	19.8
972	CB	HIS	A	943	5.232	22.971	43.767	1.00	21.85
973	CG	HIS	A	943	4.26	21.877	43.457	1.00	23.86
974	ND1	HIS	A	943	4.24	21.224	42.243	1.00	24.97
975	CD2	HIS	A	943	3.273	21.322	44.199	1.00	24.45
976	CE1	HIS	A	943	3.282	20.314	42.251	1.00	25.21
977	NE2	HIS	A	943	2.68	20.352	43.427	1.00	24.97
978	N	PHE	A	944	8.093	24.504	44.054	1.00	18.94
979	CA	PHE	A	944	8.934	25.666	43.756	1.00	17.8
980	C	PHE	A	944	10.161	25.146	43.008	1.00	17.38
981	O	PHE	A	944	10.585	25.72	42.006	1.00	16.79
982	CB	PHE	A	944	9.399	26.356	45.052	1.00	17.41
983	CG	PHE	A	944	8.355	27.231	45.697	1.00	17.66
984	CD1	PHE	A	944	8.375	27.45	47.071	1.00	17.62
985	CD2	PHE	A	944	7.378	27.871	44.928	1.00	18.05
986	CE1	PHE	A	944	7.444	28.293	47.679	1.00	18.47
987	CE2	PHE	A	944	6.439	28.719	45.525	1.00	18.67
988	CZ	PHE	A	944	6.473	28.93	46.904	1.00	18.48
989	N	ALA	A	945	10.734	24.059	43.515	1.00	16.44
990	CA	ALA	A	945	11.904	23.453	42.889	1.00	17.31
991	C	ALA	A	945	11.567	23.013	41.468	1.00	16.94
992	O	ALA	A	945	12.34	23.242	40.542	1.00	17.33
993	CB	ALA	A	945	12.388	22.251	43.717	1.00	16.34
994	N	ALA	A	946	10.401	22.395	41.3	1.00	17.73
995	CA	ALA	A	946	9.962	21.923	39.988	1.00	18.53
996	C	ALA	A	946	9.712	23.085	39.041	1.00	18.63
997	O	ALA	A	946	10.026	22.998	37.858	1.00	18.5
998	CB	ALA	A	946	8.699	21.082	40.124	1.00	18.05
999	N	ASP	A	947	9.137	24.164	39.564	1.00	18.78



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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

1000	CA	ASP	A	947	8.865	25.358	38.764	1.00	19.42
1001	C	ASP	A	947	10.152	25.907	38.148	1.00	19.25
1002	O	ASP	A	947	10.217	26.159	36.944	1.00	19.53
1003	CB	ASP	A	947	8.238	26.445	39.629	1.00	19.11
1004	CG	ASP	A	947	6.774	26.188	39.924	1.00	20.7
1005	OD1	ASP	A	947	6.226	26.893	40.798	1.00	20.8
1006	OD2	ASP	A	947	6.167	25.299	39.286	1.00	19.84
1007	N	VAL	A	948	11.17	26.095	38.982	1.00	19.35
1008	CA	VAL	A	948	12.453	26.615	38.518	1.00	19.7
1009	C	VAL	A	948	13.099	25.644	37.531	1.00	19.88
1010	O	VAL	A	948	13.628	26.057	36.504	1.00	20.52
1011	CB	VAL	A	948	13.409	26.878	39.705	1.00	19.16
1012	CG1	VAL	A	948	14.755	27.356	39.191	1.00	18.7
1013	CG2	VAL	A	948	12.807	27.931	40.626	1.00	18.08
1014	N	ALA	A	949	13.05	24.354	37.839	1.00	20.12
1015	CA	ALA	A	949	13.606	23.349	36.945	1.00	20.89
1016	C	ALA	A	949	12.901	23.414	35.589	1.00	21.37
1017	O	ALA	A	949	13.541	23.32	34.538	1.00	21.86
1018	CB	ALA	A	949	13.438	21.961	37.552	1.00	20.66
1019	N	ARG	A	950	11.578	23.573	35.613	1.00	22.01
1020	CA	ARG	A	950	10.803	23.649	34.376	1.00	21.84
1021	C	ARG	A	950	11.129	24.933	33.6	1.00	21.78
1022	O	ARG	A	950	11.197	24.925	32.368	1.00	21.94
1023	CB	ARG	A	950	9.3	23.587	34.681	1.00	21.83
1024	CG	ARG	A	950	8.438	23.286	33.456	1.00	21.84
1025	CD	ARG	A	950	6.948	23.251	33.777	1.00	22.44
1026	NE	ARG	A	950	6.643	22.322	34.86	1.00	22.17
1027	CZ	ARG	A	950	6.382	22.689	36.11	1.00	23.28
1028	NH1	ARG	A	950	6.124	21.768	37.03	1.00	22.7
1029	NH2	ARG	A	950	6.36	23.975	36.438	1.00	22.04
1030	N	GLY	A	951	11.328	26.032	34.321	1.00	21.71
1031	CA	GLY	A	951	11.657	27.294	33.675	1.00	20.89
1032	C	GLY	A	951	13.06	27.291	33.093	1.00	21.34
1033	O	GLY	A	951	13.31	27.889	32.042	1.00	21.59
1034	N	MET	A	952	13.991	26.627	33.771	1.00	21.17
1035	CA	MET	A	952	15.363	26.562	33.275	1.00	21.67
1036	C	MET	A	952	15.47	25.601	32.09	1.00	21.85
1037	O	MET	A	952	16.32	25.771	31.224	1.00	21.29
1038	CB	MET	A	952	16.332	26.138	34.384	1.00	21.53
1039	CG	MET	A	952	16.725	27.271	35.323	1.00	22.18

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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

1040	SD	MET	A	952	17.254	28.794	34.467	1.00	23.86
1041	CE	MET	A	952	18.902	28.337	33.894	1.00	21.85
1042	N	ASP	A	953	14.608	24.593	32.056	1.00	22.46
1043	CA	ASP	A	953	14.602	23.649	30.947	1.00	23.34
1044	C	ASP	A	953	14.217	24.462	29.711	1.00	23.48
1045	O	ASP	A	953	14.839	24.349	28.657	1.00	22.88
1046	CB	ASP	A	953	13.564	22.56	31.2	1.00	25.6
1047	CG	ASP	A	953	13.483	21.544	30.072	1.00	28.12
1048	OD1	ASP	A	953	12.438	20.873	29.971	1.00	30.02
1049	OD2	ASP	A	953	14.452	21.406	29.296	1.00	29.05
1050	N	TYR	A	954	13.19	25.299	29.86	1.00	23.51
1051	CA	TYR	A	954	12.719	26.156	28.776	1.00	23.6
1052	C	TYR	A	954	13.791	27.146	28.323	1.00	23.52
1053	O	TYR	A	954	14.104	27.226	27.136	1.00	24.11
1054	CB	TYR	A	954	11.485	26.941	29.225	1.00	24.17
1055	CG	TYR	A	954	11.076	28.042	28.266	1.00	25.24
1056	CD1	TYR	A	954	10.277	27.771	27.155	1.00	25.26
1057	CD2	TYR	A	954	11.483	29.358	28.477	1.00	25.38
1058	CE1	TYR	A	954	9.889	28.787	26.282	1.00	25.51
1059	CE2	TYR	A	954	11.101	30.382	27.609	1.00	25.37
1060	CZ	TYR	A	954	10.301	30.088	26.517	1.00	25.94
1061	OH	TYR	A	954	9.896	31.101	25.678	1.00	25.86
1062	N	LEU	A	955	14.339	27.907	29.267	1.00	23.47
1063	CA	LEU	A	955	15.364	28.908	28.959	1.00	24.26
1064	C	LEU	A	955	16.62	28.275	28.4	1.00	25.4
1065	O	LEU	A	955	17.215	28.783	27.452	1.00	25.65
1066	CB	LEU	A	955	15.727	29.72	30.208	1.00	23.24
1067	CG	LEU	A	955	14.633	30.613	30.792	1.00	22.47
1068	CD1	LEU	A	955	15.175	31.345	31.996	1.00	21.93
1069	CD2	LEU	A	955	14.151	31.6	29.742	1.00	23.23
1070	N	SER	A	956	17.02	27.168	29.012	1.00	27.22
1071	CA	SER	A	956	18.197	26.414	28.605	1.00	29.54
1072	C	SER	A	956	18.123	26.051	27.116	1.00	30.93
1073	O	SER	A	956	19.076	26.271	26.364	1.00	31.11
1074	CB	SER	A	956	18.287	25.142	29.458	1.00	29.27
1075	OG	SER	A	956	19.299	24.266	29.007	1.00	32.71
1076	N	GLN	A	957	16.981	25.506	26.701	1.00	31.99
1077	CA	GLN	A	957	16.77	25.093	25.316	1.00	33.56
1078	C	GLN	A	957	16.765	26.254	24.329	1.00	33.1
1079	O	GLN	A	957	17.04	26.065	23.145	1.00	33.01

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TABLE 5  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

1080	CB	GLN	A	957	15.462	24.309	25.191	1.00	35.43
1081	CG	GLN	A	957	15.472	22.965	25.907	1.00	39.2
1082	CD	GLN	A	957	14.12	22.26	25.855	1.00	42.26
1083	OE1	GLN	A	957	13.951	21.171	26.415	1.00	44.08
1084	NE2	GLN	A	957	13.148	22.881	25.186	1.00	43.09
1085	N	LYS	A	958	16.449	27.448	24.813	1.00	32.37
1086	CA	LYS	A	958	16.436	28.628	23.963	1.00	32.29
1087	C	LYS	A	958	17.825	29.265	23.997	1.00	31.7
1088	O	LYS	A	958	18.009	30.412	23.586	1.00	31.95
1089	CB	LYS	A	958	15.388	29.622	24.461	1.00	33.26
1090	CG	LYS	A	958	14.015	29.002	24.656	1.00	35.12
1091	CD	LYS	A	958	13.118	29.19	23.458	1.00	36.41
1092	CE	LYS	A	958	12.52	30.588	23.439	1.00	37.67
1093	NZ	LYS	A	958	11.471	30.716	22.384	1.00	38.7
1094	N	GLN	A	959	18.792	28.514	24.514	1.00	30.5
1095	CA	GLN	A	959	20.179	28.962	24.601	1.00	30.24
1096	C	GLN	A	959	20.533	30.04	25.631	1.00	29.21
1097	O	GLN	A	959	21.529	30.743	25.471	1.00	29.86
1098	CB	GLN	A	959	20.658	29.411	23.219	1.00	30.83
1099	CG	GLN	A	959	20.649	28.296	22.198	1.00	31.59
1100	CD	GLN	A	959	21.506	27.131	22.631	1.00	31.91
1101	OE1	GLN	A	959	22.721	27.26	22.763	1.00	32.75
1102	NE2	GLN	A	959	20.878	25.986	22.868	1.00	32.94
1103	N	PHE	A	960	19.742	30.182	26.687	1.00	27.38
1104	CA	PHE	A	960	20.082	31.176	27.696	1.00	25.77
1105	C	PHE	A	960	20.967	30.557	28.774	1.00	24.66
1106	O	PHE	A	960	20.906	29.351	29.016	1.00	23.52
1107	CB	PHE	A	960	18.826	31.758	28.355	1.00	26.37
1108	CG	PHE	A	960	18.049	32.694	27.47	1.00	26.34
1109	CD1	PHE	A	960	17.129	32.203	26.551	1.00	26.03
1110	CD2	PHE	A	960	18.236	34.067	27.563	1.00	26.48
1111	CE1	PHE	A	960	16.401	33.064	25.737	1.00	26.86
1112	CE2	PHE	A	960	17.515	34.938	26.754	1.00	26.76
1113	CZ	PHE	A	960	16.594	34.435	25.839	1.00	26.64
1114	N	ILE	A	961	21.801	31.395	29.391	1.00	23.63
1115	CA	ILE	A	961	22.691	31.002	30.482	1.00	23.31
1116	C	ILE	A	961	22.403	32.045	31.551	1.00	23.55
1117	O	ILE	A	961	22.62	33.234	31.33	1.00	23.39
1118	CB	ILE	A	961	24.181	31.094	30.091	1.00	23.28
1119	CG1	ILE	A	961	24.464	30.192	28.886	1.00	23.2

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TABLE 5  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

1120	CG2	ILE	A	961	25.051	30.697	31.287	1.00	22.19
1121	CD1	ILE	A	961	25.91	30.242	28.403	1.00	23.81
1122	N	HIS	A	962	21.921	31.608	32.71	1.00	23.56
1123	CA	HIS	A	962	21.555	32.546	33.764	1.00	24.51
1124	C	HIS	A	962	22.689	33.269	34.479	1.00	25.68
1125	O	HIS	A	962	22.66	34.495	34.597	1.00	26.4
1126	CB	HIS	A	962	20.659	31.855	34.791	1.00	23.05
1127	CG	HIS	A	962	19.899	32.812	35.654	1.00	22.28
1128	ND1	HIS	A	962	20.504	33.585	36.621	1.00	22.65
1129	CD2	HIS	A	962	18.59	33.158	35.659	1.00	21.63
1130	CE1	HIS	A	962	19.601	34.368	37.184	1.00	21.65
1131	NE2	HIS	A	962	18.432	34.129	36.617	1.00	21.35
1132	N	ARG	A	963	23.669	32.519	34.971	1.00	26.19
1133	CA	ARG	A	963	24.825	33.09	35.674	1.00	27.71
1134	C	ARG	A	963	24.621	33.353	37.165	1.00	27.26
1135	O	ARG	A	963	25.594	33.457	37.905	1.00	27.69
1136	CB	ARG	A	963	25.306	34.395	35.015	1.00	28.69
1137	CG	ARG	A	963	25.818	34.258	33.587	1.00	30.67
1138	CD	ARG	A	963	26.829	35.363	33.271	1.00	32.2
1139	NE	ARG	A	963	26.372	36.672	33.739	1.00	33.6
1140	CZ	ARG	A	963	25.346	37.345	33.221	1.00	35.25
1141	NH1	ARG	A	963	24.656	36.844	32.199	1.00	34.53
1142	NH2	ARG	A	963	24.998	38.52	33.737	1.00	35.54
1143	N	ASP	A	964	23.375	33.484	37.612	1.00	26.91
1144	CA	ASP	A	964	23.132	33.713	39.032	1.00	26.09
1145	C	ASP	A	964	21.808	33.121	39.49	1.00	24.9
1146	O	ASP	A	964	20.956	33.808	40.059	1.00	24.1
1147	CB	ASP	A	964	23.189	35.208	39.36	1.00	27.09
1148	CG	ASP	A	964	23.191	35.475	40.863	1.00	29.78
1149	OD1	ASP	A	964	23.625	34.588	41.64	1.00	29.03
1150	OD2	ASP	A	964	22.771	36.579	41.269	1.00	31.32
1151	N	LEU	A	965	21.648	31.828	39.24	1.00	23.88
1152	CA	LEU	A	965	20.443	31.121	39.626	1.00	23.73
1153	C	LEU	A	965	20.486	30.915	41.139	1.00	23.29
1154	O	LEU	A	965	21.258	30.102	41.643	1.00	24.59
1155	CB	LEU	A	965	20.387	29.782	38.892	1.00	24.49
1156	CG	LEU	A	965	19.067	29.017	38.83	1.00	25.53
1157	CD1	LEU	A	965	17.956	29.907	38.291	1.00	25.37
1158	CD2	LEU	A	965	19.252	27.803	37.938	1.00	25.6
1159	N	ALA	A	966	19.668	31.676	41.856	1.00	21.72

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## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

1160	CA	ALA	A	966	19.602	31.603	43.306	1.00	20.57
1161	C	ALA	A	966	18.207	32.028	43.731	1.00	20.68
1162	O	ALA	A	966	17.479	32.638	42.953	1.00	20.62
1163	CB	ALA	A	966	20.643	32.526	43.925	1.00	19.92
1164	N	ALA	A	967	17.836	31.709	44.965	1.00	20.58
1165	CA	ALA	A	967	16.515	32.056	45.468	1.00	20.32
1166	C	ALA	A	967	16.216	33.55	45.367	1.00	20.22
1167	O	ALA	A	967	15.07	33.947	45.146	1.00	19.34
1168	CB	ALA	A	967	16.367	31.579	46.913	1.00	20.01
1169	N	ARG	A	968	17.24	34.383	45.509	1.00	20.59
1170	CA	ARG	A	968	17.029	35.826	45.43	1.00	21.54
1171	C	ARG	A	968	16.576	36.264	44.038	1.00	20.88
1172	O	ARG	A	968	15.979	37.331	43.884	1.00	20.75
1173	CB	ARG	A	968	18.297	36.586	45.829	1.00	23.81
1174	CG	ARG	A	968	19.472	36.382	44.893	1.00	25.59
1175	CD	ARG	A	968	20.553	37.401	45.185	1.00	29.05
1176	NE	ARG	A	968	21.673	37.305	44.252	1.00	32.89
1177	CZ	ARG	A	968	22.606	38.243	44.106	1.00	34.9
1178	NH1	ARG	A	968	22.555	39.353	44.832	1.00	35.79
1179	NH2	ARG	A	968	23.593	38.072	43.237	1.00	35.71
1180	N	ASN	A	969	16.85	35.439	43.029	1.00	20
1181	CA	ASN	A	969	16.439	35.746	41.657	1.00	19.76
1182	C	ASN	A	969	15.234	34.952	41.169	1.00	19.55
1183	O	ASN	A	969	15.012	34.824	39.961	1.00	19.71
1184	CB	ASN	A	969	17.596	35.552	40.674	1.00	19.61
1185	CG	ASN	A	969	18.566	36.699	40.711	1.00	20.35
1186	OD1	ASN	A	969	18.154	37.846	40.847	1.00	21.13
1187	ND2	ASN	A	969	19.855	36.406	40.586	1.00	19.84
1188	N	ILE	A	970	14.472	34.4	42.104	1.00	18.84
1189	CA	ILE	A	970	13.255	33.668	41.76	1.00	18.63
1190	C	ILE	A	970	12.146	34.461	42.444	1.00	18.77
1191	O	ILE	A	970	12.288	34.847	43.599	1.00	18.54
1192	CB	ILE	A	970	13.233	32.222	42.335	1.00	17.93
1193	CG1	ILE	A	970	14.451	31.412	41.853	1.00	16.88
1194	CG2	ILE	A	970	11.927	31.549	41.942	1.00	16.86
1195	CD1	ILE	A	970	14.555	31.21	40.335	1.00	16.92
1196	N	LEU	A	971	11.054	34.724	41.736	1.00	18.89
1197	CA	LEU	A	971	9.951	35.469	42.335	1.00	19.27
1198	C	LEU	A	971	8.751	34.565	42.55	1.00	18.97
1199	O	LEU	A	971	8.519	33.649	41.772	1.00	19.62

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TABLE 5  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

1200	CB	LEU	A	971	9.572	36.656	41.443	1.00	19.88
1201	CG	LEU	A	971	10.753	37.631	41.327	1.00	22.07
1202	CD1	LEU	A	971	10.683	38.361	40.034	1.00	23.12
1203	CD2	LEU	A	971	10.771	38.586	42.517	1.00	21.69
1204	N	VAL	A	972	8.003	34.81	43.621	1.00	18.82
1205	CA	VAL	A	972	6.818	34.016	43.908	1.00	18.53
1206	C	VAL	A	972	5.634	34.787	43.325	1.00	19.07
1207	O	VAL	A	972	5.122	35.729	43.94	1.00	18.99
1208	CB	VAL	A	972	6.636	33.819	45.424	1.00	18.52
1209	CG1	VAL	A	972	5.437	32.938	45.692	1.00	17.52
1210	CG2	VAL	A	972	7.904	33.221	46.028	1.00	18.03
1211	N	GLY	A	973	5.219	34.38	42.126	1.00	19.17
1212	CA	GLY	A	973	4.134	35.048	41.428	1.00	19.92
1213	C	GLY	A	973	2.704	34.695	41.792	1.00	20.68
1214	O	GLY	A	973	2.44	34.113	42.84	1.00	19.71
1215	N	GLU	A	974	1.78	35.073	40.911	1.00	22.21
1216	CA	GLU	A	974	0.36	34.816	41.112	1.00	24.37
1217	C	GLU	A	974	0.154	33.337	41.363	1.00	23.72
1218	O	GLU	A	974	0.754	32.506	40.679	1.00	22.67
1219	CB	GLU	A	974	-0.448	35.213	39.873	1.00	26.68
1220	CG	GLU	A	974	-0.448	36.696	39.534	1.00	31.74
1221	CD	GLU	A	974	-1.227	37.541	40.53	1.00	34.47
1222	OE1	GLU	A	974	-2.039	36.972	41.299	1.00	36.05
1223	OE2	GLU	A	974	-1.036	38.783	40.53	1.00	36.72
1224	N	ASN	A	975	-0.702	33.021	42.333	1.00	23.88
1225	CA	ASN	A	975	-1.013	31.64	42.683	1.00	23.9
1226	C	ASN	A	975	0.222	30.888	43.154	1.00	23.54
1227	O	ASN	A	975	0.286	29.668	43.069	1.00	24.11
1228	CB	ASN	A	975	-1.639	30.932	41.48	1.00	24.94
1229	CG	ASN	A	975	-2.953	31.563	41.059	1.00	25.87
1230	OD1	ASN	A	975	-3.328	31.527	39.888	1.00	26.87
1231	ND2	ASN	A	975	-3.662	32.138	42.019	1.00	26.26
1232	N	TYR	A	976	1.195	31.639	43.656	1.00	23.47
1233	CA	TYR	A	976	2.45	31.101	44.165	1.00	22.85
1234	C	TYR	A	976	3.244	30.256	43.176	1.00	23.04
1235	O	TYR	A	976	3.85	29.255	43.546	1.00	24.02
1236	CB	TYR	A	976	2.211	30.317	45.46	1.00	22.02
1237	CG	TYR	A	976	1.6	31.171	46.55	1.00	21.37
1238	CD1	TYR	A	976	0.219	31.357	46.63	1.00	21.43
1239	CD2	TYR	A	976	2.407	31.855	47.455	1.00	20.99

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TABLE 5  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

1240	CE1	TYR	A	976	-0.338	32.206	47.583	1.00	21.15
1241	CE2	TYR	A	976	1.863	32.703	48.404	1.00	20.94
1242	CZ	TYR	A	976	0.489	32.874	48.464	1.00	21.79
1243	OH	TYR	A	976	-0.051	33.707	49.412	1.00	21.73
1244	N	VAL	A	977	3.242	30.663	41.913	1.00	21.97
1245	CA	VAL	A	977	4.012	29.953	40.898	1.00	20.74
1246	C	VAL	A	977	5.376	30.642	40.899	1.00	20.46
1247	O	VAL	A	977	5.445	31.872	40.855	1.00	19.36
1248	CB	VAL	A	977	3.366	30.086	39.492	1.00	20.36
1249	CG1	VAL	A	977	4.299	29.51	38.43	1.00	20.2
1250	CG2	VAL	A	977	2.011	29.365	39.466	1.00	19.8
1251	N	ALA	A	978	6.448	29.859	40.976	1.00	19.65
1252	CA	ALA	A	978	7.801	30.409	40.985	1.00	19.32
1253	C	ALA	A	978	8.197	30.881	39.593	1.00	19.54
1254	O	ALA	A	978	7.979	30.181	38.605	1.00	18.91
1255	CB	ALA	A	978	8.793	29.365	41.481	1.00	19.6
1256	N	LYS	A	979	8.799	32.064	39.522	1.00	18.98
1257	CA	LYS	A	979	9.214	32.629	38.247	1.00	19.45
1258	C	LYS	A	979	10.659	33.122	38.271	1.00	18.79
1259	O	LYS	A	979	11.063	33.861	39.165	1.00	18.79
1260	CB	LYS	A	979	8.257	33.759	37.865	1.00	20.53
1261	CG	LYS	A	979	6.832	33.247	37.661	1.00	21.82
1262	CD	LYS	A	979	5.841	34.362	37.426	1.00	23.17
1263	CE	LYS	A	979	4.414	33.829	37.452	1.00	24.31
1264	NZ	LYS	A	979	4.074	32.997	36.265	1.00	24.09
1265	N	ILE	A	980	11.429	32.701	37.274	1.00	18.83
1266	CA	ILE	A	980	12.845	33.054	37.165	1.00	18.2
1267	C	ILE	A	980	13.07	34.475	36.647	1.00	18.36
1268	O	ILE	A	980	12.628	34.808	35.55	1.00	17.93
1269	CB	ILE	A	980	13.561	32.086	36.206	1.00	17.48
1270	CG1	ILE	A	980	13.38	30.652	36.689	1.00	17.73
1271	CG2	ILE	A	980	15.056	32.427	36.112	1.00	17.03
1272	CD1	ILE	A	980	13.931	29.614	35.709	1.00	16.87
1273	N	ALA	A	981	13.751	35.304	37.434	1.00	18.32
1274	CA	ALA	A	981	14.065	36.672	37.019	1.00	19.29
1275	C	ALA	A	981	14.979	36.491	35.81	1.00	20.31
1276	O	ALA	A	981	16.009	35.822	35.895	1.00	20.78
1277	CB	ALA	A	981	14.791	37.413	38.132	1.00	18.31
1278	N	ASP	A	982	14.608	37.093	34.689	1.00	21.49
1279	CA	ASP	A	982	15.359	36.925	33.454	1.00	22.4

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TABLE 5  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

1280	C	ASP	A	982	15.91	38.184	32.794	1.00	22.74
1281	O	ASP	A	982	15.849	38.32	31.575	1.00	22.11
1282	CB	ASP	A	982	14.469	36.18	32.464	1.00	22.85
1283	CG	ASP	A	982	13.066	36.752	32.413	1.00	23.58
1284	OD1	ASP	A	982	12.154	36.072	31.894	1.00	24.5
1285	OD2	ASP	A	982	12.873	37.888	32.894	1.00	23.62
1286	N	PHE	A	983	16.448	39.098	33.591	1.00	23.82
1287	CA	PHE	A	983	17.013	40.326	33.047	1.00	25.06
1288	C	PHE	A	983	18.536	40.225	32.995	1.00	25.47
1289	O	PHE	A	983	19.166	39.769	33.951	1.00	25.4
1290	CB	PHE	A	983	16.624	41.522	33.914	1.00	25.67
1291	CG	PHE	A	983	16.984	42.844	33.306	1.00	26.67
1292	CD1	PHE	A	983	16.187	43.407	32.316	1.00	27.36
1293	CD2	PHE	A	983	18.14	43.51	33.693	1.00	27.48
1294	CE1	PHE	A	983	16.538	44.612	31.718	1.00	27.68
1295	CE2	PHE	A	983	18.5	44.719	33.097	1.00	28.05
1296	CZ	PHE	A	983	17.696	45.268	32.108	1.00	27.94
1297	N	GLY	A	984	19.122	40.645	31.877	1.00	26.22
1298	CA	GLY	A	984	20.569	40.609	31.734	1.00	27.03
1299	C	GLY	A	984	21.207	39.227	31.684	1.00	27.66
1300	O	GLY	A	984	22.293	39.027	32.231	1.00	27.85
1301	N	LEU	A	985	20.548	38.277	31.023	1.00	27.4
1302	CA	LEU	A	985	21.071	36.919	30.91	1.00	27.55
1303	C	LEU	A	985	21.962	36.806	29.686	1.00	28.22
1304	O	LEU	A	985	21.905	37.652	28.801	1.00	28.33
1305	CB	LEU	A	985	19.926	35.913	30.769	1.00	26.75
1306	CG	LEU	A	985	18.804	35.98	31.803	1.00	26.71
1307	CD1	LEU	A	985	17.812	34.864	31.535	1.00	26.09
1308	CD2	LEU	A	985	19.391	35.862	33.209	1.00	26.23
1309	N	SER	A	986	22.779	35.758	29.644	1.00	28.49
1310	CA	SER	A	986	23.669	35.509	28.515	1.00	29.35
1311	C	SER	A	986	22.986	34.511	27.591	1.00	29.77
1312	O	SER	A	986	22.009	33.874	27.976	1.00	29.72
1313	CB	SER	A	986	24.998	34.909	28.986	1.00	28.93
1314	OG	SER	A	986	25.71	35.803	29.822	1.00	30.06
1315	N	ARG	A	987	23.5	34.371	26.374	1.00	30.41
1316	CA	ARG	A	987	22.927	33.424	25.433	1.00	31.16
1317	C	ARG	A	987	24.018	32.797	24.585	1.00	30.3
1318	O	ARG	A	987	24.801	33.496	23.956	1.00	30.64
1319	CB	ARG	A	987	21.886	34.115	24.545	1.00	33.19



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TABLE 5  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

1320	CG	ARG	A	987	20.57	33.347	24.462	1.00	34.93
1321	CD	ARG	A	987	19.465	34.177	23.826	1.00	36.22
1322	NE	ARG	A	987	19.727	34.455	22.42	1.00	37.02
1323	CZ	ARG	A	987	19.479	33.61	21.427	1.00	37.11
1324	NH1	ARG	A	987	18.954	32.419	21.678	1.00	36.7
1325	NH2	ARG	A	987	19.756	33.962	20.178	1.00	38.63
1326	N	GLY	A	988	24.069	31.471	24.581	1.00	29.7
1327	CA	GLY	A	988	25.075	30.773	23.808	1.00	29.6
1328	C	GLY	A	988	25.449	29.462	24.463	1.00	29.79
1329	O	GLY	A	988	24.723	28.963	25.32	1.00	29.44
1330	N	GLN	A	989	26.579	28.895	24.057	1.00	29.6
1331	CA	GLN	A	989	27.036	27.639	24.629	1.00	30.19
1332	C	GLN	A	989	27.798	27.905	25.919	1.00	29.09
1333	O	GLN	A	989	27.627	27.203	26.911	1.00	29.13
1334	CB	GLN	A	989	27.963	26.923	23.655	1.00	32.59
1335	CG	GLN	A	989	28.495	25.595	24.169	1.00	36.52
1336	CD	GLN	A	989	29.675	25.095	23.353	1.00	39.49
1337	OE1	GLN	A	989	30.096	23.941	23.48	1.00	41.88
1338	NE2	GLN	A	989	30.225	25.967	22.517	1.00	40.57
1339	N	GLU	A	990	28.647	28.923	25.892	1.00	27.9
1340	CA	GLU	A	990	29.458	29.266	27.044	1.00	27.36
1341	C	GLU	A	990	29.758	30.753	27.066	1.00	27.09
1342	O	GLU	A	990	29.943	31.38	26.025	1.00	26.66
1343	CB	GLU	A	990	30.769	28.476	27.006	1.00	26.65
1344	CG	GLU	A	990	31.736	28.787	28.136	1.00	26.68
1345	CD	GLU	A	990	32.973	27.897	28.095	1.00	27.62
1346	OE1	GLU	A	990	33.761	28.024	27.141	1.00	28
1347	OE2	GLU	A	990	33.154	27.062	29.004	1.00	28.24
1348	N	VAL	A	991	29.8	31.315	28.264	1.00	27.02
1349	CA	VAL	A	991	30.088	32.727	28.413	1.00	27.83
1350	C	VAL	A	991	31.239	32.956	29.389	1.00	27.59
1351	O	VAL	A	991	31.312	32.327	30.445	1.00	27.19
1352	CB	VAL	A	991	28.832	33.497	28.889	1.00	28.23
1353	CG1	VAL	A	991	29.158	34.965	29.084	1.00	29.36
1354	CG2	VAL	A	991	27.733	33.362	27.85	1.00	29.29
1355	N	TYR	A	992	32.15	33.841	29.001	1.00	27.57
1356	CA	TYR	A	992	33.295	34.193	29.825	1.00	28.39
1357	C	TYR	A	992	33.074	35.614	30.325	1.00	29.54
1358	O	TYR	A	992	32.933	36.549	29.534	1.00	28.89
1359	CB	TYR	A	992	34.589	34.142	29.008	1.00	28.34

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TABLE 5  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

1360	CG	TYR	A	992	35.796	34.698	29.741	1.00	27.73
1361	CD1	TYR	A	992	36.378	33.998	30.795	1.00	27.53
1362	CD2	TYR	A	992	36.345	35.933	29.389	1.00	27.63
1363	CE1	TYR	A	992	37.477	34.512	31.48	1.00	27.69
1364	CE2	TYR	A	992	37.446	36.455	30.068	1.00	27.23
1365	CZ	TYR	A	992	38.004	35.739	31.113	1.00	27.53
1366	OH	TYR	A	992	39.075	36.248	31.807	1.00	28.03
1367	N	VAL	A	993	33.042	35.775	31.64	1.00	31.18
1368	CA	VAL	A	993	32.834	37.083	32.236	1.00	33.85
1369	C	VAL	A	993	33.891	37.336	33.308	1.00	36.12
1370	O	VAL	A	993	33.816	36.78	34.4	1.00	36.39
1371	CB	VAL	A	993	31.432	37.177	32.884	1.00	33.13
1372	CG1	VAL	A	993	31.239	38.547	33.512	1.00	32.74
1373	CG2	VAL	A	993	30.356	36.904	31.844	1.00	32.43
1374	N	LYS	A	994	34.882	38.166	33.001	1.00	39.01
1375	CA	LYS	A	994	35.915	38.459	33.987	1.00	42.29
1376	C	LYS	A	994	35.278	39.199	35.159	1.00	43.91
1377	O	LYS	A	994	34.492	40.12	34.951	1.00	44.66
1378	CB	LYS	A	994	37.024	39.321	33.383	1.00	42.33
1379	CG	LYS	A	994	38.141	39.587	34.372	1.00	43.51
1380	CD	LYS	A	994	39.079	40.69	33.927	1.00	44.48
1381	CE	LYS	A	994	39.984	40.25	32.804	1.00	44.62
1382	NZ	LYS	A	994	41.046	41.268	32.588	1.00	45.83
1383	N	ALA	A	995	35.62	38.789	36.381	1.00	46.13
1384	CA	ALA	A	995	35.083	39.392	37.607	1.00	48.36
1385	C	ALA	A	995	34.48	40.781	37.387	1.00	49.89
1386	O	ALA	A	995	33.265	40.967	37.523	1.00	50.59
1387	CB	ALA	A	995	36.173	39.461	38.675	1.00	47.87
1388	N	ALA	A	996	35.336	41.745	37.043	1.00	51.26
1389	CA	ALA	A	996	34.922	43.127	36.793	1.00	52.23
1390	CB	ALA	A	996	33.674	43.159	35.902	1.00	52.31
1391	C	ALA	A	996	34.662	43.884	38.092	1.00	52.8
1392	OT1	ALA	A	996	35.046	43.367	39.164	1.00	53.26
1393	OT2	ALA	A	996	34.087	44.992	38.02	1.00	53.2
1394	N	ALA	A	999	30.973	41.023	45.137	1.00	39.75
1395	CA	ALA	A	999	30.739	41.465	43.731	1.00	39.35
1396	C	ALA	A	999	30.372	40.272	42.851	1.00	38.9
1397	O	ALA	A	999	29.812	40.432	41.764	1.00	39.83
1398	CB	ALA	A	999	31.993	42.154	43.187	1.00	39.67
1399	N	LEU	A	0	30.691	39.077	43.335	1.00	37.57

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TABLE 5  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

1400	CA	LEU	A	0	30.42	37.846	42.607	1.00	35.54
1401	C	LEU	A	0	29.698	36.891	43.557	1.00	33.74
1402	O	LEU	A	0	30.047	36.81	44.733	1.00	33.52
1403	CB	LEU	A	0	31.747	37.233	42.157	1.00	36.17
1404	CG	LEU	A	0	31.843	36.438	40.855	1.00	37.03
1405	CD1	LEU	A	0	31.467	37.311	39.669	1.00	36.11
1406	CD2	LEU	A	0	33.275	35.935	40.699	1.00	38.02
1407	N	PRO	A	1	28.679	36.163	43.061	1.00	31.83
1408	CA	PRO	A	1	27.902	35.207	43.863	1.00	30.72
1409	C	PRO	A	1	28.633	33.874	44.057	1.00	29.53
1410	O	PRO	A	1	28.125	32.81	43.707	1.00	29.1
1411	CB	PRO	A	1	26.625	35.054	43.049	1.00	30
1412	CG	PRO	A	1	27.15	35.107	41.648	1.00	30.35
1413	CD	PRO	A	1	28.109	36.282	41.705	1.00	31.06
1414	N	VAL	A	2	29.831	33.954	44.619	1.00	28.77
1415	CA	VAL	A	2	30.684	32.796	44.87	1.00	28.44
1416	C	VAL	A	2	30.007	31.549	45.437	1.00	27.78
1417	O	VAL	A	2	30.239	30.432	44.972	1.00	27.63
1418	CB	VAL	A	2	31.829	33.178	45.839	1.00	29.31
1419	CG1	VAL	A	2	32.704	31.966	46.122	1.00	29.91
1420	CG2	VAL	A	2	32.647	34.317	45.248	1.00	29.69
1421	N	ARG	A	3	29.177	31.735	46.45	1.00	27.12
1422	CA	ARG	A	3	28.526	30.609	47.095	1.00	26.99
1423	C	ARG	A	3	27.562	29.818	46.21	1.00	26.22
1424	O	ARG	A	3	27.147	28.72	46.572	1.00	26.22
1425	CB	ARG	A	3	27.84	31.115	48.365	1.00	28.48
1426	CG	ARG	A	3	28.78	31.991	49.195	1.00	29.77
1427	CD	ARG	A	3	28.097	32.631	50.384	1.00	31.4
1428	NE	ARG	A	3	28.369	31.891	51.608	1.00	34.03
1429	CZ	ARG	A	3	29.366	32.151	52.447	1.00	32.77
1430	NH1	ARG	A	3	30.208	33.148	52.217	1.00	32.66
1431	NH2	ARG	A	3	29.524	31.396	53.52	1.00	34.58
1432	N	TRP	A	4	27.224	30.366	45.045	1.00	25.43
1433	CA	TRP	A	4	26.317	29.705	44.099	1.00	24.17
1434	C	TRP	A	4	27.04	29.282	42.818	1.00	24.14
1435	O	TRP	A	4	26.439	28.668	41.941	1.00	23.73
1436	CB	TRP	A	4	25.176	30.653	43.701	1.00	22.75
1437	CG	TRP	A	4	24.082	30.777	44.715	1.00	21.85
1438	CD1	TRP	A	4	22.909	30.083	44.739	1.00	21.66
1439	CD2	TRP	A	4	24.073	31.625	45.871	1.00	21.45

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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

1440	NE1	TRP	A	4	22.167	30.442	45.841	1.00	22.09
1441	CE2	TRP	A	4	22.858	31.386	46.554	1.00	21.52
1442	CE3	TRP	A	4	24.974	32.56	46.397	1.00	20.99
1443	CZ2	TRP	A	4	22.518	32.05	47.74	1.00	20.7
1444	CZ3	TRP	A	4	24.635	33.223	47.581	1.00	21.28
1445	CH2	TRP	A	4	23.417	32.961	48.236	1.00	20.6
1446	N	MET	A	5	28.325	29.611	42.713	1.00	24.01
1447	CA	MET	A	5	29.099	29.313	41.505	1.00	24.05
1448	C	MET	A	5	29.763	27.945	41.422	1.00	23.51
1449	O	MET	A	5	30.34	27.459	42.393	1.00	23.51
1450	CB	MET	A	5	30.161	30.399	41.304	1.00	25.03
1451	CG	MET	A	5	29.594	31.757	40.925	1.00	26.54
1452	SD	MET	A	5	30.786	33.081	41.152	1.00	29.37
1453	CE	MET	A	5	32.068	32.588	39.95	1.00	28.39
1454	N	ALA	A	6	29.679	27.334	40.244	1.00	23.42
1455	CA	ALA	A	6	30.283	26.024	40.003	1.00	24.19
1456	C	ALA	A	6	31.81	26.143	40.036	1.00	23.98
1457	O	ALA	A	6	32.365	27.221	39.824	1.00	23.06
1458	CB	ALA	A	6	29.827	25.473	38.642	1.00	24.05
1459	N	ILE	A	7	32.486	25.032	40.299	1.00	25.08
1460	CA	ILE	A	7	33.944	25.038	40.359	1.00	26.01
1461	C	ILE	A	7	34.576	25.631	39.097	1.00	25.63
1462	O	ILE	A	7	35.487	26.446	39.185	1.00	26.42
1463	CB	ILE	A	7	34.491	23.616	40.582	1.00	26.85
1464	CG1	ILE	A	7	33.981	23.078	41.92	1.00	27.64
1465	CG2	ILE	A	7	36.019	23.634	40.566	1.00	27.48
1466	CD1	ILE	A	7	34.414	21.651	42.234	1.00	28.78
1467	N	GLU	A	8	34.092	25.236	37.925	1.00	25.84
1468	CA	GLU	A	8	34.653	25.759	36.684	1.00	25.55
1469	C	GLU	A	8	34.468	27.27	36.585	1.00	25.13
1470	O	GLU	A	8	35.278	27.955	35.965	1.00	24.65
1471	CB	GLU	A	8	34.015	25.082	35.469	1.00	25.55
1472	CG	GLU	A	8	32.536	25.359	35.309	1.00	26.9
1473	CD	GLU	A	8	31.665	24.261	35.885	1.00	27.7
1474	OE1	GLU	A	8	32.064	23.646	36.898	1.00	28.76
1475	OE2	GLU	A	8	30.572	24.022	35.329	1.00	27.45
1476	N	SER	A	9	33.401	27.789	37.192	1.00	24.63
1477	CA	SER	A	9	33.138	29.23	37.166	1.00	24.81
1478	C	SER	A	9	34.054	29.97	38.136	1.00	25.27
1479	O	SER	A	9	34.497	31.083	37.864	1.00	24.62

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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

1480	CB	SER	A	9	31.677	29.523	37.525	1.00	24.64
1481	OG	SER	A	9	30.785	28.926	36.597	1.00	24.78
1482	N	LEU	A	10	34.33	29.356	39.278	1.00	25.64
1483	CA	LEU	A	10	35.203	29.985	40.253	1.00	26.4
1484	C	LEU	A	10	36.6	30.047	39.655	1.00	26.88
1485	O	LEU	A	10	37.288	31.066	39.756	1.00	26.51
1486	CB	LEU	A	10	35.221	29.174	41.554	1.00	26.28
1487	CG	LEU	A	10	33.895	29.129	42.324	1.00	26.36
1488	CD1	LEU	A	10	33.945	28.08	43.413	1.00	26.61
1489	CD2	LEU	A	10	33.615	30.496	42.918	1.00	26.47
1490	N	ASN	A	11	36.992	28.958	38.998	1.00	27.25
1491	CA	ASN	A	11	38.318	28.855	38.396	1.00	27.52
1492	C	ASN	A	11	38.58	29.674	37.148	1.00	27.03
1493	O	ASN	A	11	39.586	30.38	37.066	1.00	27.31
1494	CB	ASN	A	11	38.644	27.394	38.058	1.00	28.29
1495	CG	ASN	A	11	38.843	26.543	39.283	1.00	29.56
1496	OD1	ASN	A	11	39.246	27.039	40.333	1.00	31.01
1497	ND2	ASN	A	11	38.581	25.249	39.155	1.00	29.28
1498	N	TYR	A	12	37.679	29.587	36.176	1.00	26.28
1499	CA	TYR	A	12	37.897	30.261	34.903	1.00	25.5
1500	C	TYR	A	12	36.897	31.327	34.472	1.00	25.54
1501	O	TYR	A	12	36.956	31.806	33.338	1.00	25.37
1502	CB	TYR	A	12	38.001	29.196	33.81	1.00	25.42
1503	CG	TYR	A	12	38.822	27.993	34.221	1.00	24.87
1504	CD1	TYR	A	12	38.236	26.731	34.356	1.00	24.85
1505	CD2	TYR	A	12	40.187	28.118	34.487	1.00	25.21
1506	CE1	TYR	A	12	38.996	25.618	34.75	1.00	25.76
1507	CE2	TYR	A	12	40.953	27.021	34.881	1.00	25.46
1508	CZ	TYR	A	12	40.356	25.778	35.012	1.00	26
1509	OH	TYR	A	12	41.124	24.711	35.421	1.00	26.87
1510	N	SER	A	13	35.979	31.693	35.36	1.00	24.55
1511	CA	SER	A	13	34.982	32.712	35.047	1.00	24.19
1512	C	SER	A	13	34.117	32.394	33.825	1.00	23.08
1513	O	SER	A	13	33.686	33.302	33.116	1.00	22.3
1514	CB	SER	A	13	35.66	34.069	34.837	1.00	24.28
1515	OG	SER	A	13	36.438	34.425	35.964	1.00	26.93
1516	N	VAL	A	14	33.86	31.111	33.584	1.00	22.63
1517	CA	VAL	A	14	33.029	30.707	32.463	1.00	21.75
1518	C	VAL	A	14	31.688	30.211	32.995	1.00	22.77
1519	O	VAL	A	14	31.605	29.686	34.108	1.00	23.14

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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

1520	CB	VAL	A	14	33.698	29.583	31.628	1.00	22.55
1521	CG1	VAL	A	14	35.02	30.087	31.039	1.00	22.05
1522	CG2	VAL	A	14	33.928	28.343	32.49	1.00	21.17
1523	N	TYR	A	15	30.64	30.392	32.199	1.00	22.67
1524	CA	TYR	A	15	29.298	29.974	32.584	1.00	22.54
1525	C	TYR	A	15	28.615	29.215	31.448	1.00	22.38
1526	O	TYR	A	15	28.708	29.607	30.28	1.00	22.32
1527	CB	TYR	A	15	28.448	31.2	32.955	1.00	21.64
1528	CG	TYR	A	15	29.019	32.022	34.083	1.00	21.65
1529	CD1	TYR	A	15	30.051	32.939	33.86	1.00	22.77
1530	CD2	TYR	A	15	28.539	31.875	35.379	1.00	21.01
1531	CE1	TYR	A	15	30.587	33.698	34.92	1.00	22.52
1532	CE2	TYR	A	15	29.064	32.613	36.438	1.00	21.41
1533	CZ	TYR	A	15	30.082	33.522	36.208	1.00	22.42
1534	OH	TYR	A	15	30.581	34.249	37.27	1.00	22.38
1535	N	THR	A	16	27.929	28.136	31.809	1.00	21.85
1536	CA	THR	A	16	27.203	27.297	30.859	1.00	22.54
1537	C	THR	A	16	25.912	26.801	31.513	1.00	22.84
1538	O	THR	A	16	25.621	27.133	32.663	1.00	22.43
1539	CB	THR	A	16	28.017	26.055	30.471	1.00	22.52
1540	OG1	THR	A	16	28.207	25.238	31.636	1.00	21.2
1541	CG2	THR	A	16	29.375	26.453	29.886	1.00	22.32
1542	N	THR	A	17	25.139	26.01	30.776	1.00	23.2
1543	CA	THR	A	17	23.909	25.449	31.315	1.00	23.38
1544	C	THR	A	17	24.32	24.501	32.427	1.00	23.75
1545	O	THR	A	17	23.631	24.379	33.439	1.00	23.7
1546	CB	THR	A	17	23.127	24.678	30.243	1.00	23.51
1547	OG1	THR	A	17	22.653	25.604	29.266	1.00	24.6
1548	CG2	THR	A	17	21.927	23.95	30.849	1.00	23.85
1549	N	ASN	A	18	25.459	23.838	32.239	1.00	24.24
1550	CA	ASN	A	18	25.962	22.917	33.247	1.00	24.78
1551	C	ASN	A	18	26.285	23.66	34.549	1.00	23.89
1552	O	ASN	A	18	26.013	23.145	35.629	1.00	23.95
1553	CB	ASN	A	18	27.202	22.163	32.742	1.00	25.98
1554	CG	ASN	A	18	26.859	21.08	31.722	1.00	27.8
1555	OD1	ASN	A	18	25.868	20.359	31.868	1.00	28.69
1556	ND2	ASN	A	18	27.69	20.952	30.695	1.00	28.39
1557	N	SER	A	19	26.856	24.862	34.462	1.00	23.56
1558	CA	SER	A	19	27.153	25.603	35.688	1.00	22.93
1559	C	SER	A	19	25.855	26.135	36.288	1.00	22.54

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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

1560	O	SER	A	19	25.779	26.367	37.492	1.00	23.04
1561	CB	SER	A	19	28.152	26.747	35.447	1.00	22.42
1562	OG	SER	A	19	27.662	27.749	34.576	1.00	23.13
1563	N	ASP	A	20	24.831	26.318	35.453	1.00	22.53
1564	CA	ASP	A	20	23.526	26.777	35.941	1.00	21.98
1565	C	ASP	A	20	22.915	25.651	36.78	1.00	21.86
1566	O	ASP	A	20	22.238	25.897	37.772	1.00	21.75
1567	CB	ASP	A	20	22.576	27.113	34.78	1.00	21.52
1568	CG	ASP	A	20	22.71	28.556	34.298	1.00	22.89
1569	OD1	ASP	A	20	23.373	29.367	34.98	1.00	23.37
1570	OD2	ASP	A	20	22.135	28.888	33.237	1.00	23.07
1571	N	VAL	A	21	23.163	24.41	36.373	1.00	22.68
1572	CA	VAL	A	21	22.642	23.261	37.099	1.00	22.33
1573	C	VAL	A	21	23.282	23.209	38.486	1.00	22.74
1574	O	VAL	A	21	22.632	22.835	39.465	1.00	23.14
1575	CB	VAL	A	21	22.921	21.951	36.329	1.00	22.21
1576	CG1	VAL	A	21	22.63	20.737	37.21	1.00	21.78
1577	CG2	VAL	A	21	22.052	21.9	35.074	1.00	22.13
1578	N	TRP	A	22	24.555	23.583	38.574	1.00	22.45
1579	CA	TRP	A	22	25.232	23.592	39.866	1.00	22.71
1580	C	TRP	A	22	24.518	24.618	40.733	1.00	22.25
1581	O	TRP	A	22	24.15	24.327	41.868	1.00	22.93
1582	CB	TRP	A	22	26.709	23.973	39.713	1.00	22.59
1583	CG	TRP	A	22	27.449	24.112	41.022	1.00	23.09
1584	CD1	TRP	A	22	27.232	25.044	41.996	1.00	22.44
1585	CD2	TRP	A	22	28.563	23.323	41.465	1.00	23.55
1586	NE1	TRP	A	22	28.141	24.888	43.016	1.00	23.12
1587	CE2	TRP	A	22	28.97	23.841	42.714	1.00	23.36
1588	CE3	TRP	A	22	29.257	22.233	40.925	1.00	23.53
1589	CZ2	TRP	A	22	30.046	23.305	43.432	1.00	23.79
1590	CZ3	TRP	A	22	30.325	21.7	41.639	1.00	24.58
1591	CH2	TRP	A	22	30.708	22.239	42.88	1.00	24.28
1592	N	SER	A	23	24.332	25.822	40.201	1.00	21.9
1593	CA	SER	A	23	23.637	26.864	40.951	1.00	22.37
1594	C	SER	A	23	22.249	26.369	41.353	1.00	21.62
1595	O	SER	A	23	21.82	26.572	42.489	1.00	22.39
1596	CB	SER	A	23	23.508	28.136	40.12	1.00	22.11
1597	OG	SER	A	23	24.786	28.621	39.768	1.00	23.64
1598	N	TYR	A	24	21.556	25.715	40.426	1.00	20.46
1599	CA	TYR	A	24	20.232	25.185	40.716	1.00	20.21

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TABLE 5  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

1600	C	TYR	A	24	20.303	24.301	41.954	1.00	20.44
1601	O	TYR	A	24	19.44	24.368	42.826	1.00	20.39
1602	CB	TYR	A	24	19.697	24.343	39.551	1.00	20.04
1603	CG	TYR	A	24	18.355	23.715	39.87	1.00	19.74
1604	CD1	TYR	A	24	17.179	24.463	39.797	1.00	19.84
1605	CD2	TYR	A	24	18.27	22.403	40.34	1.00	19.96
1606	CE1	TYR	A	24	15.948	23.923	40.191	1.00	20.04
1607	CE2	TYR	A	24	17.049	21.854	40.745	1.00	20.15
1608	CZ	TYR	A	24	15.894	22.619	40.669	1.00	20.32
1609	OH	TYR	A	24	14.695	22.094	41.095	1.00	20.14
1610	N	GLY	A	25	21.33	23.457	42.015	1.00	20.27
1611	CA	GLY	A	25	21.491	22.577	43.158	1.00	20.42
1612	C	GLY	A	25	21.551	23.374	44.451	1.00	20.74
1613	O	GLY	A	25	20.957	22.991	45.458	1.00	20.22
1614	N	VAL	A	26	22.281	24.485	44.422	1.00	20.72
1615	CA	VAL	A	26	22.392	25.347	45.59	1.00	20.85
1616	C	VAL	A	26	21.022	25.968	45.888	1.00	21.1
1617	O	VAL	A	26	20.641	26.105	47.055	1.00	21.4
1618	CB	VAL	A	26	23.447	26.468	45.365	1.00	21.21
1619	CG1	VAL	A	26	23.497	27.4	46.576	1.00	20.41
1620	CG2	VAL	A	26	24.83	25.844	45.136	1.00	20.07
1621	N	LEU	A	27	20.281	26.322	44.835	1.00	20.41
1622	CA	LEU	A	27	18.95	26.91	44.992	1.00	20.61
1623	C	LEU	A	27	18.018	25.918	45.679	1.00	20.29
1624	O	LEU	A	27	17.208	26.294	46.528	1.00	20.52
1625	CB	LEU	A	27	18.362	27.302	43.63	1.00	20.98
1626	CG	LEU	A	27	16.832	27.443	43.582	1.00	22.73
1627	CD1	LEU	A	27	16.365	28.491	44.578	1.00	24
1628	CD2	LEU	A	27	16.396	27.814	42.178	1.00	24.64
1629	N	LEU	A	28	18.127	24.65	45.3	1.00	19.75
1630	CA	LEU	A	28	17.304	23.606	45.896	1.00	19.52
1631	C	LEU	A	28	17.662	23.501	47.383	1.00	19.77
1632	O	LEU	A	28	16.795	23.281	48.228	1.00	19.08
1633	CB	LEU	A	28	17.547	22.272	45.18	1.00	19.52
1634	CG	LEU	A	28	16.825	21.026	45.709	1.00	19.2
1635	CD1	LEU	A	28	15.329	21.254	45.705	1.00	19.33
1636	CD2	LEU	A	28	17.173	19.822	44.841	1.00	19.93
1637	N	TRP	A	29	18.945	23.671	47.699	1.00	19.61
1638	CA	TRP	A	29	19.383	23.622	49.09	1.00	19.72
1639	C	TRP	A	29	18.732	24.788	49.852	1.00	18.6



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TABLE 5  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

1640	O	TRP	A	29	18.279	24.622	50.981	1.00	19.11
1641	CB	TRP	A	29	20.914	23.72	49.176	1.00	19.59
1642	CG	TRP	A	29	21.46	23.533	50.574	1.00	20.28
1643	CD1	TRP	A	29	21.838	22.359	51.157	1.00	19.63
1644	CD2	TRP	A	29	21.675	24.559	51.559	1.00	19.68
1645	NE1	TRP	A	29	22.281	22.588	52.44	1.00	20.85
1646	CE2	TRP	A	29	22.188	23.927	52.713	1.00	20.41
1647	CE3	TRP	A	29	21.481	25.949	51.576	1.00	19.35
1648	CZ2	TRP	A	29	22.512	24.637	53.878	1.00	19.93
1649	CZ3	TRP	A	29	21.805	26.657	52.736	1.00	19.43
1650	CH2	TRP	A	29	22.314	25.996	53.87	1.00	20.47
1651	N	GLU	A	30	18.679	25.965	49.232	1.00	18.55
1652	CA	GLU	A	30	18.05	27.121	49.875	1.00	19.24
1653	C	GLU	A	30	16.564	26.863	50.15	1.00	19.19
1654	O	GLU	A	30	16.035	27.241	51.198	1.00	19.6
1655	CB	GLU	A	30	18.151	28.358	48.996	1.00	19.49
1656	CG	GLU	A	30	19.538	28.846	48.736	1.00	20.63
1657	CD	GLU	A	30	19.523	30.083	47.881	1.00	21.65
1658	OE1	GLU	A	30	19.413	31.196	48.446	1.00	21.14
1659	OE2	GLU	A	30	19.599	29.934	46.639	1.00	21.44
1660	N	ILE	A	31	15.891	26.239	49.192	1.00	18.15
1661	CA	ILE	A	31	14.473	25.942	49.343	1.00	18.53
1662	C	ILE	A	31	14.245	25.01	50.526	1.00	19.02
1663	O	ILE	A	31	13.483	25.32	51.447	1.00	18.69
1664	CB	ILE	A	31	13.91	25.279	48.063	1.00	17.04
1665	CG1	ILE	A	31	13.808	26.326	46.947	1.00	16.99
1666	CG2	ILE	A	31	12.561	24.611	48.357	1.00	15.93
1667	CD1	ILE	A	31	13.3	25.773	45.627	1.00	15.39
1668	N	VAL	A	32	14.918	23.868	50.489	1.00	19.59
1669	CA	VAL	A	32	14.796	22.872	51.538	1.00	20.98
1670	C	VAL	A	32	15.165	23.412	52.919	1.00	21.3
1671	O	VAL	A	32	14.548	23.033	53.916	1.00	22.02
1672	CB	VAL	A	32	15.673	21.652	51.214	1.00	21.45
1673	CG1	VAL	A	32	15.64	20.659	52.357	1.00	22.7
1674	CG2	VAL	A	32	15.182	21.008	49.94	1.00	21.3
1675	N	SER	A	33	16.16	24.297	52.977	1.00	21.32
1676	CA	SER	A	33	16.607	24.865	54.248	1.00	20.68
1677	C	SER	A	33	15.841	26.133	54.623	1.00	20.67
1678	O	SER	A	33	16.259	26.885	55.504	1.00	20.51
1679	CB	SER	A	33	18.106	25.172	54.195	1.00	20.65

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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

1680	OG	SER	A	33	18.373	26.321	53.409	1.00	22.44
1681	N	LEU	A	34	14.725	26.374	53.942	1.00	19.88
1682	CA	LEU	A	34	13.894	27.537	54.22	1.00	19.45
1683	C	LEU	A	34	14.647	28.875	54.171	1.00	19.41
1684	O	LEU	A	34	14.491	29.729	55.042	1.00	19.1
1685	CB	LEU	A	34	13.206	27.355	55.581	1.00	19.1
1686	CG	LEU	A	34	12.379	26.057	55.705	1.00	19
1687	CD1	LEU	A	34	11.922	25.827	57.144	1.00	18.87
1688	CD2	LEU	A	34	11.188	26.134	54.769	1.00	18.5
1689	N	GLY	A	35	15.477	29.048	53.151	1.00	19.52
1690	CA	GLY	A	35	16.194	30.299	53.005	1.00	20.42
1691	C	GLY	A	35	17.509	30.438	53.738	1.00	20.8
1692	O	GLY	A	35	17.925	31.554	54.056	1.00	20.35
1693	N	GLY	A	36	18.168	29.319	54.012	1.00	21.23
1694	CA	GLY	A	36	19.444	29.394	54.695	1.00	22.43
1695	C	GLY	A	36	20.528	29.888	53.752	1.00	23.31
1696	O	GLY	A	36	20.408	29.752	52.531	1.00	22.42
1697	N	THR	A	37	21.574	30.485	54.318	1.00	23.38
1698	CA	THR	A	37	22.705	30.981	53.54	1.00	23.99
1699	C	THR	A	37	23.639	29.785	53.345	1.00	24.05
1700	O	THR	A	37	24.037	29.134	54.314	1.00	23.69
1701	CB	THR	A	37	23.455	32.095	54.303	1.00	25
1702	OG1	THR	A	37	22.576	33.212	54.505	1.00	26.12
1703	CG2	THR	A	37	24.69	32.551	53.525	1.00	24.75
1704	N	PRO	A	38	24.004	29.479	52.089	1.00	24.21
1705	CA	PRO	A	38	24.89	28.341	51.817	1.00	24.37
1706	C	PRO	A	38	26.277	28.509	52.441	1.00	24.43
1707	O	PRO	A	38	26.839	29.599	52.417	1.00	23.2
1708	CB	PRO	A	38	24.959	28.308	50.287	1.00	24.53
1709	CG	PRO	A	38	23.714	29.033	49.853	1.00	24.96
1710	CD	PRO	A	38	23.652	30.169	50.839	1.00	24.14
1711	N	TYR	A	39	26.821	27.429	52.993	1.00	25.29
1712	CA	TYR	A	39	28.152	27.473	53.603	1.00	27.03
1713	C	TYR	A	39	28.211	28.512	54.72	1.00	28.35
1714	O	TYR	A	39	29.238	29.165	54.923	1.00	28.11
1715	CB	TYR	A	39	29.209	27.817	52.543	1.00	26.36
1716	CG	TYR	A	39	29.107	27.003	51.271	1.00	25.37
1717	CD1	TYR	A	39	29.464	25.653	51.249	1.00	25.13
1718	CD2	TYR	A	39	28.642	27.581	50.087	1.00	25.34
1719	CE1	TYR	A	39	29.362	24.9	50.08	1.00	24.99

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TABLE 5  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

1720	CE2	TYR	A	39	28.531	26.833	48.905	1.00	24.29
1721	CZ	TYR	A	39	28.894	25.494	48.911	1.00	25.3
1722	OH	TYR	A	39	28.789	24.746	47.755	1.00	25.24
1723	N	CYS	A	40	27.102	28.678	55.432	1.00	30.34
1724	CA	CYS	A	40	27.051	29.632	56.526	1.00	32.29
1725	C	CYS	A	40	28.129	29.175	57.496	1.00	34.05
1726	O	CYS	A	40	28.23	27.987	57.796	1.00	34.19
1727	CB	CYS	A	40	25.681	29.584	57.21	1.00	32.51
1728	SG	CYS	A	40	25.348	30.961	58.334	1.00	33.86
1729	N	GLY	A	41	28.95	30.097	57.971	1.00	35.48
1730	CA	GLY	A	41	29.988	29.693	58.9	1.00	38.38
1731	C	GLY	A	41	31.313	29.409	58.226	1.00	40.13
1732	O	GLY	A	41	32.292	29.076	58.892	1.00	40.81
1733	N	MET	A	42	31.343	29.522	56.901	1.00	41.43
1734	CA	MET	A	42	32.565	29.309	56.131	1.00	42.69
1735	C	MET	A	42	32.865	30.59	55.369	1.00	43.55
1736	O	MET	A	42	31.959	31.229	54.838	1.00	43.7
1737	CB	MET	A	42	32.398	28.158	55.134	1.00	43.09
1738	CG	MET	A	42	32.439	26.769	55.749	1.00	43.95
1739	SD	MET	A	42	32.233	25.448	54.517	1.00	45.46
1740	CE	MET	A	42	33.819	25.519	53.677	1.00	44.31
1741	N	THR	A	43	34.135	30.973	55.325	1.00	44.56
1742	CA	THR	A	43	34.532	32.177	54.606	1.00	45.82
1743	C	THR	A	43	34.651	31.812	53.134	1.00	46.67
1744	O	THR	A	43	34.726	30.632	52.791	1.00	46.62
1745	CB	THR	A	43	35.9	32.682	55.081	1.00	45.63
1746	OG1	THR	A	43	36.91	31.738	54.702	1.00	45.7
1747	CG2	THR	A	43	35.913	32.841	56.59	1.00	45.53
1748	N	CYS	A	44	34.662	32.811	52.26	1.00	48.04
1749	CA	CYS	A	44	34.797	32.533	50.839	1.00	49.64
1750	C	CYS	A	44	36.125	31.813	50.618	1.00	50.35
1751	O	CYS	A	44	36.199	30.838	49.87	1.00	50.21
1752	CB	CYS	A	44	34.741	33.831	50.03	1.00	49.94
1753	SG	CYS	A	44	33.086	34.586	49.992	1.00	51.97
1754	N	ALA	A	45	37.169	32.28	51.295	1.00	51.11
1755	CA	ALA	A	45	38.479	31.66	51.173	1.00	52.12
1756	C	ALA	A	45	38.378	30.17	51.482	1.00	52.67
1757	O	ALA	A	45	38.84	29.336	50.705	1.00	53.16
1758	CB	ALA	A	45	39.463	32.327	52.12	1.00	52.45
1759	N	GLU	A	46	37.769	29.837	52.616	1.00	53.3

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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

1760	CA	GLU	A	46	37.609	28.441	53.013	1.00	54.15
1761	C	GLU	A	46	36.853	27.668	51.934	1.00	54.6
1762	O	GLU	A	46	37.046	26.461	51.764	1.00	54.21
1763	CB	GLU	A	46	36.849	28.344	54.341	1.00	54.6
1764	CG	GLU	A	46	37.563	28.974	55.528	1.00	55.41
1765	CD	GLU	A	46	36.763	28.872	56.822	1.00	56.2
1766	OE1	GLU	A	46	35.629	29.393	56.871	1.00	56.34
1767	OE2	GLU	A	46	37.271	28.271	57.793	1.00	56.52
1768	N	LEU	A	47	35.99	28.379	51.21	1.00	55.17
1769	CA	LEU	A	47	35.196	27.783	50.14	1.00	55.37
1770	C	LEU	A	47	36.089	27.378	48.978	1.00	55.41
1771	O	LEU	A	47	36.147	26.206	48.612	1.00	55.11
1772	CB	LEU	A	47	34.142	28.774	49.637	1.00	55.36
1773	CG	LEU	A	47	32.661	28.414	49.788	1.00	55.63
1774	CD1	LEU	A	47	31.832	29.399	48.976	1.00	55.49
1775	CD2	LEU	A	47	32.402	26.994	49.307	1.00	55.27
1776	N	TYR	A	48	36.777	28.36	48.398	1.00	56.09
1777	CA	TYR	A	48	37.671	28.108	47.273	1.00	56.5
1778	C	TYR	A	48	38.634	26.981	47.592	1.00	55.88
1779	O	TYR	A	48	39.045	26.236	46.711	1.00	55.81
1780	CB	TYR	A	48	38.49	29.351	46.93	1.00	57.74
1781	CG	TYR	A	48	37.688	30.507	46.393	1.00	59.48
1782	CD1	TYR	A	48	36.98	31.341	47.249	1.00	60.28
1783	CD2	TYR	A	48	37.65	30.776	45.024	1.00	60.1
1784	CE1	TYR	A	48	36.255	32.42	46.767	1.00	60.9
1785	CE2	TYR	A	48	36.924	31.855	44.526	1.00	61.3
1786	CZ	TYR	A	48	36.231	32.673	45.408	1.00	61.54
1787	OH	TYR	A	48	35.518	33.75	44.935	1.00	62.7
1788	N	GLU	A	49	38.991	26.866	48.864	1.00	55.69
1789	CA	GLU	A	49	39.917	25.834	49.298	1.00	55.34
1790	C	GLU	A	49	39.274	24.452	49.363	1.00	54.13
1791	O	GLU	A	49	39.771	23.499	48.767	1.00	54.06
1792	CB	GLU	A	49	40.487	26.198	50.67	1.00	56.75
1793	CG	GLU	A	49	41.646	25.322	51.109	1.00	58.94
1794	CD	GLU	A	49	42.112	25.636	52.518	1.00	60.28
1795	OE1	GLU	A	49	42.407	26.821	52.799	1.00	60.97
1796	OE2	GLU	A	49	42.187	24.698	53.342	1.00	61.15
1797	N	LYS	A	50	38.16	24.35	50.079	1.00	52.69
1798	CA	LYS	A	50	37.475	23.076	50.243	1.00	51.22
1799	C	LYS	A	50	36.687	22.535	49.051	1.00	50.49

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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

1800	O	LYS	A	50	36.608	21.32	48.867	1.00	50.15
1801	CB	LYS	A	50	36.561	23.139	51.467	1.00	51.5
1802	CG	LYS	A	50	37.267	22.842	52.781	1.00	51.64
1803	CD	LYS	A	50	36.261	22.671	53.904	1.00	51.97
1804	CE	LYS	A	50	36.771	21.72	54.974	1.00	52.6
1805	NZ	LYS	A	50	38.03	22.204	55.606	1.00	53.32
1806	N	LEU	A	51	36.1	23.412	48.244	1.00	49.44
1807	CA	LEU	A	51	35.32	22.948	47.1	1.00	48.68
1808	C	LEU	A	51	36.079	21.988	46.185	1.00	48.25
1809	O	LEU	A	51	35.607	20.887	45.905	1.00	48.04
1810	CB	LEU	A	51	34.786	24.136	46.293	1.00	48.66
1811	CG	LEU	A	51	33.537	24.806	46.879	1.00	48.5
1812	CD1	LEU	A	51	33.159	26.026	46.048	1.00	48.33
1813	CD2	LEU	A	51	32.39	23.804	46.913	1.00	47.61
1814	N	PRO	A	52	37.269	22.387	45.71	1.00	48.07
1815	CA	PRO	A	52	38.035	21.501	44.83	1.00	47.53
1816	C	PRO	A	52	38.446	20.214	45.544	1.00	46.88
1817	O	PRO	A	52	38.73	19.202	44.906	1.00	47.17
1818	CB	PRO	A	52	39.232	22.36	44.445	1.00	47.85
1819	CG	PRO	A	52	39.46	23.164	45.688	1.00	48.36
1820	CD	PRO	A	52	38.051	23.589	46.046	1.00	48.36
1821	N	GLN	A	53	38.473	20.261	46.871	1.00	45.88
1822	CA	GLN	A	53	38.843	19.097	47.666	1.00	45.08
1823	C	GLN	A	53	37.694	18.105	47.744	1.00	43.76
1824	O	GLN	A	53	37.823	17.037	48.346	1.00	44.06
1825	CB	GLN	A	53	39.249	19.523	49.079	1.00	45.94
1826	CG	GLN	A	53	40.527	20.342	49.125	1.00	47.31
1827	CD	GLN	A	53	40.904	20.763	50.532	1.00	48.56
1828	OE1	GLN	A	53	41.94	21.396	50.744	1.00	49.54
1829	NE2	GLN	A	53	40.062	20.418	51.503	1.00	49.03
1830	N	GLY	A	54	36.567	18.464	47.14	1.00	41.87
1831	CA	GLY	A	54	35.419	17.576	47.154	1.00	39.75
1832	C	GLY	A	54	34.354	17.93	48.172	1.00	38.33
1833	O	GLY	A	54	33.366	17.212	48.307	1.00	37.65
1834	N	TYR	A	55	34.544	19.032	48.891	1.00	37.2
1835	CA	TYR	A	55	33.566	19.451	49.884	1.00	36.75
1836	C	TYR	A	55	32.287	19.965	49.216	1.00	36.04
1837	O	TYR	A	55	32.342	20.637	48.187	1.00	36.25
1838	CB	TYR	A	55	34.156	20.543	50.792	1.00	37.45
1839	CG	TYR	A	55	33.204	20.983	51.878	1.00	38.13

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TABLE 5  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

1840	CD1	TYR	A	55	32.175	21.886	51.606	1.00	38.32
1841	CD2	TYR	A	55	33.264	20.419	53.15	1.00	38.54
1842	CE1	TYR	A	55	31.225	22.207	52.565	1.00	38.75
1843	CE2	TYR	A	55	32.317	20.731	54.121	1.00	39
1844	CZ	TYR	A	55	31.296	21.624	53.82	1.00	39.38
1845	OH	TYR	A	55	30.33	21.915	54.759	1.00	39.07
1846	N	ARG	A	56	31.141	19.643	49.811	1.00	34.84
1847	CA	ARG	A	56	29.837	20.07	49.295	1.00	33.92
1848	C	ARG	A	56	28.886	20.374	50.453	1.00	33.7
1849	O	ARG	A	56	29.098	19.911	51.572	1.00	33.69
1850	CB	ARG	A	56	29.227	18.972	48.42	1.00	33.11
1851	CG	ARG	A	56	30.058	18.597	47.197	1.00	32.11
1852	CD	ARG	A	56	29.986	19.653	46.112	1.00	30.42
1853	NE	ARG	A	56	30.582	19.173	44.866	1.00	29.93
1854	CZ	ARG	A	56	31.885	19.179	44.603	1.00	29.88
1855	NH1	ARG	A	56	32.747	19.647	45.502	1.00	28.4
1856	NH2	ARG	A	56	32.328	18.722	43.436	1.00	29.11
1857	N	LEU	A	57	27.84	21.152	50.185	1.00	33.21
1858	CA	LEU	A	57	26.862	21.492	51.214	1.00	32.37
1859	C	LEU	A	57	26.328	20.226	51.381	1.00	32.71
1860	O	LEU	A	57	25.962	19.259	51.21	1.00	31.87
1861	CB	LEU	A	57	25.695	22.268	50.601	1.00	31.27
1862	CG	LEU	A	57	25.975	23.675	50.069	1.00	30.83
1863	CD1	LEU	A	57	24.829	24.107	49.166	1.00	30.22
1864	CD2	LEU	A	57	26.156	24.649	51.238	1.00	29.57
1865	N	GLU	A	58	26.283	20.237	53.206	1.00	33.27
1866	CA	GLU	A	58	25.781	19.09	53.947	1.00	34.43
1867	C	GLU	A	58	24.27	19.008	53.798	1.00	33.59
1868	O	GLU	A	58	23.628	19.979	53.401	1.00	33.28
1869	CB	GLU	A	58	26.175	19.206	55.419	1.00	36.49
1870	CG	GLU	A	58	27.681	19.056	55.643	1.00	40.09
1871	CD	GLU	A	58	28.068	19.02	57.116	1.00	42.19
1872	OE1	GLU	A	58	29.233	18.665	57.411	1.00	44.21
1873	OE2	GLU	A	58	27.215	19.346	57.974	1.00	42.66
1874	N	LYS	A	59	23.7	17.849	54.106	1.00	33
1875	CA	LYS	A	59	22.26	17.675	53.978	1.00	33.15
1876	C	LYS	A	59	21.465	18.257	55.137	1.00	32.52
1877	O	LYS	A	59	21.74	17.953	56.296	1.00	32.93
1878	CB	LYS	A	59	21.898	16.199	53.85	1.00	33.47
1879	CG	LYS	A	59	20.413	16.001	53.618	1.00	34.91

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TABLE 5  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

1880	CD	LYS	A	59	20.004	14.542	53.602	1.00	36
1881	CE	LYS	A	59	19.994	13.961	55	1.00	37.12
1882	NZ	LYS	A	59	19.359	12.619	55.018	1.00	38.54
1883	N	PRO	A	60	20.471	19.114	54.838	1.00	32.11
1884	CA	PRO	A	60	19.65	19.71	55.899	1.00	31.12
1885	C	PRO	A	60	18.976	18.576	56.678	1.00	30.83
1886	O	PRO	A	60	18.525	17.594	56.086	1.00	29.94
1887	CB	PRO	A	60	18.642	20.546	55.122	1.00	31.35
1888	CG	PRO	A	60	19.419	20.969	53.903	1.00	31.71
1889	CD	PRO	A	60	20.146	19.699	53.522	1.00	31.68
1890	N	LEU	A	61	18.911	18.707	57.999	1.00	30.92
1891	CA	LEU	A	61	18.302	17.676	58.835	1.00	30.96
1892	C	LEU	A	61	16.843	17.37	58.509	1.00	30.5
1893	O	LEU	A	61	16.347	16.293	58.828	1.00	30.67
1894	CB	LEU	A	61	18.419	18.062	60.31	1.00	31.59
1895	CG	LEU	A	61	19.846	18.222	60.834	1.00	32.62
1896	CD1	LEU	A	61	19.818	18.605	62.303	1.00	32.76
1897	CD2	LEU	A	61	20.607	16.92	60.639	1.00	33.66
1898	N	ASN	A	62	16.156	18.307	57.869	1.00	29.95
1899	CA	ASN	A	62	14.749	18.109	57.526	1.00	29.42
1900	C	ASN	A	62	14.599	17.579	56.1	1.00	30.18
1901	O	ASN	A	62	13.487	17.357	55.621	1.00	29.84
1902	CB	ASN	A	62	13.999	19.434	57.662	1.00	28.21
1903	CG	ASN	A	62	14.41	20.444	56.608	1.00	27.34
1904	OD1	ASN	A	62	15.599	20.669	56.373	1.00	26.89
1905	ND2	ASN	A	62	13.424	21.063	55.969	1.00	26.7
1906	N	CYS	A	63	15.726	17.368	55.432	1.00	31.1
1907	CA	CYS	A	63	15.718	16.892	54.059	1.00	33.14
1908	C	CYS	A	63	15.853	15.378	53.91	1.00	34.17
1909	O	CYS	A	63	16.648	14.738	54.594	1.00	34.09
1910	CB	CYS	A	63	16.836	17.582	53.283	1.00	32.59
1911	SG	CYS	A	63	16.876	17.178	51.554	1.00	33.19
1912	N	ASP	A	64	15.063	14.812	53.005	1.00	35.76
1913	CA	ASP	A	64	15.094	13.378	52.739	1.00	37.33
1914	C	ASP	A	64	16.338	13.061	51.913	1.00	37.36
1915	O	ASP	A	64	16.915	13.952	51.29	1.00	36.87
1916	CB	ASP	A	64	13.848	12.971	51.959	1.00	39.56
1917	CG	ASP	A	64	13.803	11.498	51.674	1.00	42.02
1918	OD1	ASP	A	64	13.559	10.721	52.624	1.00	44.25
1919	OD2	ASP	A	64	14.023	11.107	50.505	1.00	43.51

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TABLE 5  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

1920	N	ASP	A	65	16.751	11.795	51.905	1.00	37.75
1921	CA	ASP	A	65	17.932	11.385	51.146	1.00	37.68
1922	C	ASP	A	65	17.787	11.552	49.639	1.00	37.02
1923	O	ASP	A	65	18.727	11.968	48.965	1.00	36.58
1924	CB	ASP	A	65	18.284	9.922	51.427	1.00	39.2
1925	CG	ASP	A	65	18.972	9.73	52.755	1.00	40.82
1926	OD1	ASP	A	65	19.857	10.545	53.095	1.00	42.73
1927	OD2	ASP	A	65	18.64	8.753	53.453	1.00	42.04
1928	N	GLU	A	66	16.617	11.216	49.111	1.00	36.88
1929	CA	GLU	A	66	16.381	11.316	47.677	1.00	36.82
1930	C	GLU	A	66	16.558	12.752	47.187	1.00	35.59
1931	O	GLU	A	66	17.136	12.989	46.127	1.00	35.39
1932	CB	GLU	A	66	14.973	10.819	47.345	1.00	38.54
1933	CG	GLU	A	66	14.847	10.144	45.985	1.00	41.78
1934	CD	GLU	A	66	13.42	9.704	45.676	1.00	43.37
1935	OE1	GLU	A	66	12.767	9.117	46.565	1.00	44.47
1936	OE2	GLU	A	66	12.953	9.937	44.539	1.00	45.17
1937	N	VAL	A	67	16.068	13.71	47.969	1.00	34.44
1938	CA	VAL	A	67	16.176	15.116	47.6	1.00	33.03
1939	C	VAL	A	67	17.631	15.547	47.596	1.00	32.13
1940	O	VAL	A	67	18.095	16.168	46.646	1.00	32.06
1941	CB	VAL	A	67	15.372	16.027	48.567	1.00	32.84
1942	CG1	VAL	A	67	15.472	17.487	48.124	1.00	31.93
1943	CG2	VAL	A	67	13.916	15.597	48.588	1.00	32.38
1944	N	TYR	A	68	18.352	15.204	48.655	1.00	31.55
1945	CA	TYR	A	68	19.761	15.557	48.757	1.00	31.73
1946	C	TYR	A	68	20.58	14.92	47.629	1.00	32.28
1947	O	TYR	A	68	21.489	15.55	47.084	1.00	32.43
1948	CB	TYR	A	68	20.32	15.117	50.111	1.00	30.88
1949	CG	TYR	A	68	21.757	15.526	50.347	1.00	30.59
1950	CD1	TYR	A	68	22.13	16.87	50.342	1.00	30.09
1951	CD2	TYR	A	68	22.744	14.57	50.603	1.00	30.44
1952	CE1	TYR	A	68	23.449	17.255	50.591	1.00	29.92
1953	CE2	TYR	A	68	24.067	14.944	50.854	1.00	29.91
1954	CZ	TYR	A	68	24.41	16.288	50.849	1.00	30.42
1955	OH	TYR	A	68	25.705	16.67	51.13	1.00	29.58
1956	N	ASP	A	69	20.27	13.673	47.282	1.00	32.08
1957	CA	ASP	A	69	21.004	13.008	46.214	1.00	32.63
1958	C	ASP	A	69	20.905	13.841	44.942	1.00	31.84
1959	O	ASP	A	69	21.888	14.003	44.22	1.00	31.54



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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

1960	CB	ASP	A	69	20.449	11.604	45.95	1.00	33.71
1961	CG	ASP	A	69	20.665	10.661	47.119	1.00	35.38
1962	OD1	ASP	A	69	21.719	10.776	47.785	1.00	35.68
1963	OD2	ASP	A	69	19.79	9.8	47.364	1.00	36.56
1964	N	LEU	A	70	19.711	14.362	44.67	1.00	31.01
1965	CA	LEU	A	70	19.504	15.183	43.487	1.00	30.72
1966	C	LEU	A	70	20.436	16.386	43.595	1.00	30.46
1967	O	LEU	A	70	21.08	16.778	42.621	1.00	30.18
1968	CB	LEU	A	70	18.046	15.637	43.408	1.00	30.3
1969	CG	LEU	A	70	17.627	16.476	42.196	1.00	30.54
1970	CD1	LEU	A	70	17.944	15.739	40.907	1.00	30.36
1971	CD2	LEU	A	70	16.14	16.772	42.281	1.00	29.74
1972	N	MET	A	71	20.518	16.956	44.793	1.00	29.89
1973	CA	MET	A	71	21.383	18.103	45.025	1.00	29.89
1974	C	MET	A	71	22.819	17.744	44.676	1.00	30.08
1975	O	MET	A	71	23.53	18.522	44.034	1.00	29.39
1976	CB	MET	A	71	21.332	18.531	46.494	1.00	29.24
1977	CG	MET	A	71	20.072	19.233	46.927	1.00	28.25
1978	SD	MET	A	71	20.269	19.77	48.624	1.00	28.52
1979	CE	MET	A	71	18.638	19.453	49.297	1.00	28.44
1980	N	ARG	A	72	23.239	16.562	45.116	1.00	30.46
1981	CA	ARG	A	72	24.597	16.091	44.876	1.00	31.49
1982	C	ARG	A	72	24.875	15.847	43.403	1.00	31.29
1983	O	ARG	A	72	25.959	16.163	42.919	1.00	31.07
1984	CB	ARG	A	72	24.863	14.817	45.68	1.00	32.27
1985	CG	ARG	A	72	24.85	15.038	47.186	1.00	33.34
1986	CD	ARG	A	72	25.903	16.063	47.586	1.00	34.39
1987	NE	ARG	A	72	27.252	15.611	47.256	1.00	35.81
1988	CZ	ARG	A	72	28.045	14.936	48.084	1.00	36.71
1989	NH1	ARG	A	72	27.632	14.63	49.307	1.00	36.83
1990	NH2	ARG	A	72	29.258	14.565	47.69	1.00	37.4
1991	N	GLN	A	73	23.906	15.279	42.693	1.00	31.55
1992	CA	GLN	A	73	24.08	15.033	41.268	1.00	32.24
1993	C	GLN	A	73	24.424	16.37	40.61	1.00	31.63
1994	O	GLN	A	73	25.249	16.438	39.702	1.00	31.82
1995	CB	GLN	A	73	22.791	14.493	40.643	1.00	34.21
1996	CG	GLN	A	73	22.15	13.313	41.36	1.00	37.32
1997	CD	GLN	A	73	20.82	12.902	40.724	1.00	38.93
1998	OE1	GLN	A	73	19.972	12.277	41.369	1.00	40.69
1999	NE2	GLN	A	73	20.639	13.247	39.452	1.00	39.28

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TABLE 5  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

2000	N	CYS	A	74	23.786	17.434	41.091	1.00	30.49
2001	CA	CYS	A	74	23.989	18.78	40.564	1.00	29.32
2002	C	CYS	A	74	25.382	19.351	40.787	1.00	29.37
2003	O	CYS	A	74	25.851	20.157	39.987	1.00	28.22
2004	CB	CYS	A	74	22.969	19.748	41.175	1.00	28.94
2005	SG	CYS	A	74	21.267	19.528	40.628	1.00	26.81
2006	N	TRP	A	75	26.038	18.95	41.873	1.00	29.7
2007	CA	TRP	A	75	27.368	19.469	42.177	1.00	30.64
2008	C	TRP	A	75	28.525	18.563	41.77	1.00	31.37
2009	O	TRP	A	75	29.611	18.651	42.338	1.00	31.74
2010	CB	TRP	A	75	27.495	19.795	43.67	1.00	30.15
2011	CG	TRP	A	75	26.414	20.691	44.179	1.00	30.43
2012	CD1	TRP	A	75	25.871	21.772	43.54	1.00	30.68
2013	CD2	TRP	A	75	25.732	20.581	45.433	1.00	30.5
2014	NE1	TRP	A	75	24.888	22.339	44.318	1.00	30.6
2015	CE2	TRP	A	75	24.782	21.629	45.487	1.00	30.84
2016	CE3	TRP	A	75	25.829	19.699	46.519	1.00	29.66
2017	CZ2	TRP	A	75	23.931	21.816	46.584	1.00	30.32
2018	CZ3	TRP	A	75	24.984	19.884	47.608	1.00	30.42
2019	CH2	TRP	A	75	24.048	20.936	47.633	1.00	30.18
2020	N	ARG	A	76	28.303	17.698	40.792	1.00	31.79
2021	CA	ARG	A	76	29.373	16.825	40.336	1.00	33.45
2022	C	ARG	A	76	30.495	17.672	39.751	1.00	33.45
2023	O	ARG	A	76	30.252	18.608	38.987	1.00	32.59
2024	CB	ARG	A	76	28.847	15.833	39.298	1.00	34.48
2025	CG	ARG	A	76	28.143	14.647	39.926	1.00	37.12
2026	CD	ARG	A	76	27.18	13.977	38.964	1.00	40.09
2027	NE	ARG	A	76	26.561	12.799	39.57	1.00	42.28
2028	CZ	ARG	A	76	25.435	12.234	39.143	1.00	43.42
2029	NH1	ARG	A	76	24.959	11.164	39.766	1.00	44.1
2030	NH2	ARG	A	76	24.775	12.744	38.106	1.00	43.58
2031	N	GLU	A	77	31.723	17.341	40.135	1.00	33.71
2032	CA	GLU	A	77	32.908	18.055	39.675	1.00	34.51
2033	C	GLU	A	77	32.949	18.168	38.145	1.00	33.88
2034	O	GLU	A	77	33.27	19.227	37.599	1.00	32.93
2035	CB	GLU	A	77	34.156	17.336	40.206	1.00	36.69
2036	CG	GLU	A	77	35.479	18.056	40	1.00	39.36
2037	CD	GLU	A	77	36.016	17.91	38.591	1.00	41.17
2038	OE1	GLU	A	77	35.96	16.785	38.049	1.00	42.69
2039	OE2	GLU	A	77	36.504	18.914	38.029	1.00	42.5

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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

2040	N	LYS	A	78	32.62	17.078	37.459	1.00	33.32
2041	CA	LYS	A	78	32.612	17.071	36.001	1.00	33.54
2042	C	LYS	A	78	31.265	17.579	35.484	1.00	33.15
2043	O	LYS	A	78	30.243	16.899	35.613	1.00	32.36
2044	CB	LYS	A	78	32.886	15.659	35.497	1.00	34.38
2045	CG	LYS	A	78	34.247	15.145	35.937	1.00	36.21
2046	CD	LYS	A	78	34.437	13.677	35.61	1.00	37.85
2047	CE	LYS	A	78	35.791	13.183	36.113	1.00	38.79
2048	NZ	LYS	A	78	35.981	11.73	35.838	1.00	39.72
2049	N	PRO	A	79	31.257	18.785	34.885	1.00	33.02
2050	CA	PRO	A	79	30.071	19.449	34.332	1.00	33.05
2051	C	PRO	A	79	29.134	18.539	33.557	1.00	33.7
2052	O	PRO	A	79	27.929	18.534	33.8	1.00	33.25
2053	CB	PRO	A	79	30.669	20.547	33.456	1.00	32.87
2054	CG	PRO	A	79	31.92	20.907	34.184	1.00	32.45
2055	CD	PRO	A	79	32.475	19.549	34.557	1.00	32.89
2056	N	TYR	A	80	29.692	17.764	32.63	1.00	34.56
2057	CA	TYR	A	80	28.891	16.865	31.809	1.00	35.62
2058	C	TYR	A	80	28.321	15.675	32.583	1.00	35.72
2059	O	TYR	A	80	27.58	14.868	32.027	1.00	35.71
2060	CB	TYR	A	80	29.72	16.382	30.615	1.00	37.46
2061	CG	TYR	A	80	30.995	15.673	30.997	1.00	38.59
2062	CD1	TYR	A	80	30.983	14.331	31.384	1.00	39.74
2063	CD2	TYR	A	80	32.212	16.35	31.005	1.00	39.56
2064	CE1	TYR	A	80	32.153	13.684	31.771	1.00	40.04
2065	CE2	TYR	A	80	33.388	15.712	31.392	1.00	40.29
2066	CZ	TYR	A	80	33.347	14.382	31.774	1.00	40.43
2067	OH	TYR	A	80	34.498	13.755	32.178	1.00	42.04
2068	N	GLU	A	81	28.663	15.57	33.864	1.00	35.95
2069	CA	GLU	A	81	28.151	14.486	34.699	1.00	35.75
2070	C	GLU	A	81	26.892	14.941	35.435	1.00	34.44
2071	O	GLU	A	81	26.153	14.128	36	1.00	33.95
2072	CB	GLU	A	81	29.202	14.043	35.723	1.00	37.64
2073	CG	GLU	A	81	30.351	13.233	35.147	1.00	41.07
2074	CD	GLU	A	81	29.866	12.054	34.33	1.00	42.88
2075	OE1	GLU	A	81	28.945	11.35	34.795	1.00	44.76
2076	OE2	GLU	A	81	30.406	11.824	33.227	1.00	44.88
2077	N	ARG	A	82	26.658	16.249	35.433	1.00	32.69
2078	CA	ARG	A	82	25.491	16.814	36.096	1.00	30.98
2079	C	ARG	A	82	24.263	16.534	35.249	1.00	30.39

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TABLE 5  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

2080	O	ARG	A	82	24.352	16.434	34.027	1.00	30.93
2081	CB	ARG	A	82	25.676	18.318	36.274	1.00	29.53
2082	CG	ARG	A	82	26.94	18.659	37.04	1.00	28.93
2083	CD	ARG	A	82	27.263	20.135	37.028	1.00	27.63
2084	NE	ARG	A	82	28.627	20.352	37.496	1.00	27.25
2085	CZ	ARG	A	82	29.318	21.464	37.292	1.00	27
2086	NH1	ARG	A	82	28.764	22.473	36.632	1.00	27.06
2087	NH2	ARG	A	82	30.576	21.55	37.708	1.00	25.53
2088	N	PRO	A	83	23.097	16.377	35.888	1.00	29.78
2089	CA	PRO	A	83	21.886	16.11	35.116	1.00	29.72
2090	C	PRO	A	83	21.411	17.352	34.371	1.00	29.4
2091	O	PRO	A	83	21.893	18.46	34.61	1.00	29.1
2092	CB	PRO	A	83	20.895	15.665	36.185	1.00	29.72
2093	CG	PRO	A	83	21.318	16.464	37.369	1.00	29.57
2094	CD	PRO	A	83	22.818	16.338	37.333	1.00	29.5
2095	N	SER	A	84	20.472	17.152	33.455	1.00	29.13
2096	CA	SER	A	84	19.901	18.246	32.687	1.00	28.97
2097	C	SER	A	84	18.668	18.715	33.458	1.00	28.6
2098	O	SER	A	84	18.167	17.993	34.321	1.00	28.29
2099	CB	SER	A	84	19.486	17.754	31.303	1.00	29.37
2100	OG	SER	A	84	18.507	16.736	31.412	1.00	29.08
2101	N	PHE	A	85	18.18	19.913	33.158	1.00	27.44
2102	CA	PHE	A	85	17.011	20.415	33.86	1.00	26.9
2103	C	PHE	A	85	15.8	19.529	33.603	1.00	27.13
2104	O	PHE	A	85	14.942	19.367	34.472	1.00	27.23
2105	CB	PHE	A	85	16.734	21.867	33.454	1.00	25.29
2106	CG	PHE	A	85	17.677	22.849	34.087	1.00	24
2107	CD1	PHE	A	85	17.693	23.016	35.47	1.00	23.16
2108	CD2	PHE	A	85	18.581	23.572	33.311	1.00	22.96
2109	CE1	PHE	A	85	18.599	23.889	36.077	1.00	22.76
2110	CE2	PHE	A	85	19.49	24.446	33.904	1.00	22.41
2111	CZ	PHE	A	85	19.5	24.604	35.291	1.00	23.02
2112	N	ALA	A	86	15.747	18.932	32.415	1.00	27.25
2113	CA	ALA	A	86	14.64	18.055	32.062	1.00	27.61
2114	C	ALA	A	86	14.664	16.829	32.96	1.00	27.89
2115	O	ALA	A	86	13.619	16.327	33.374	1.00	28.41
2116	CB	ALA	A	86	14.741	17.639	30.591	1.00	28.45
2117	N	GLN	A	87	15.865	16.356	33.272	1.00	27.82
2118	CA	GLN	A	87	16.008	15.185	34.123	1.00	28.22
2119	C	GLN	A	87	15.702	15.554	35.562	1.00	27.75

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TABLE 5  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

2120	O	GLN	A	87	15.087	14.779	36.296	1.00	27.59
2121	CB	GLN	A	87	17.425	14.62	34.005	1.00	29.96
2122	CG	GLN	A	87	17.782	14.201	32.587	1.00	31.74
2123	CD	GLN	A	87	19.177	13.623	32.477	1.00	33.2
2124	OE1	GLN	A	87	20.153	14.243	32.895	1.00	33.43
2125	NE2	GLN	A	87	19.277	12.43	31.901	1.00	33.94
2126	N	ILE	A	88	16.135	16.745	35.963	1.00	26.65
2127	CA	ILE	A	88	15.878	17.22	37.313	1.00	26.17
2128	C	ILE	A	88	14.371	17.301	37.512	1.00	26.23
2129	O	ILE	A	88	13.85	16.849	38.526	1.00	26.49
2130	CB	ILE	A	88	16.483	18.611	37.534	1.00	25.84
2131	CG1	ILE	A	88	18.009	18.517	37.502	1.00	25.06
2132	CG2	ILE	A	88	15.983	19.194	38.848	1.00	25
2133	CD1	ILE	A	88	18.704	19.863	37.457	1.00	24.61
2134	N	LEU	A	89	13.676	17.873	36.532	1.00	26.6
2135	CA	LEU	A	89	12.225	18.006	36.6	1.00	26.8
2136	C	LEU	A	89	11.549	16.646	36.72	1.00	27.36
2137	O	LEU	A	89	10.623	16.475	37.514	1.00	26.58
2138	CB	LEU	A	89	11.702	18.725	35.362	1.00	25.79
2139	CG	LEU	A	89	10.189	18.94	35.288	1.00	25.59
2140	CD1	LEU	A	89	9.697	19.681	36.528	1.00	24.15
2141	CD2	LEU	A	89	9.86	19.722	34.026	1.00	24.36
2142	N	VAL	A	90	12.006	15.682	35.922	1.00	28.66
2143	CA	VAL	A	90	11.446	14.332	35.965	1.00	29.32
2144	C	VAL	A	90	11.59	13.772	37.372	1.00	29.97
2145	O	VAL	A	90	10.647	13.207	37.913	1.00	30.31
2146	CB	VAL	A	90	12.164	13.366	34.99	1.00	29.3
2147	CG1	VAL	A	90	11.642	11.955	35.192	1.00	29.04
2148	CG2	VAL	A	90	11.927	13.796	33.56	1.00	29.33
2149	N	SER	A	91	12.774	13.932	37.958	1.00	31.02
2150	CA	SER	A	91	13.02	13.441	39.308	1.00	32.39
2151	C	SER	A	91	12.085	14.103	40.307	1.00	33.05
2152	O	SER	A	91	11.508	13.432	41.163	1.00	33.31
2153	CB	SER	A	91	14.466	13.703	39.734	1.00	32.35
2154	OG	SER	A	91	15.369	12.891	39.015	1.00	33.38
2155	N	LEU	A	92	11.936	15.421	40.198	1.00	33.27
2156	CA	LEU	A	92	11.074	16.154	41.115	1.00	33.44
2157	C	LEU	A	92	9.612	15.741	40.98	1.00	33.94
2158	O	LEU	A	92	8.904	15.618	41.978	1.00	33.74
2159	CB	LEU	A	92	11.231	17.661	40.898	1.00	32.66

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TABLE 5  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

2160	CG	LEU	A	92	12.583	18.226	41.351	1.00	32.68
2161	CD1	LEU	A	92	12.717	19.679	40.928	1.00	31.46
2162	CD2	LEU	A	92	12.711	18.085	42.865	1.00	31.65
2163	N	ASN	A	93	9.157	15.529	39.75	1.00	35.13
2164	CA	ASN	A	93	7.773	15.126	39.536	1.00	36.36
2165	C	ASN	A	93	7.477	13.743	40.119	1.00	37.58
2166	O	ASN	A	93	6.386	13.51	40.634	1.00	37.92
2167	CB	ASN	A	93	7.417	15.156	38.043	1.00	35.62
2168	CG	ASN	A	93	7.241	16.573	37.515	1.00	35.57
2169	OD1	ASN	A	93	6.866	17.48	38.262	1.00	35.26
2170	ND2	ASN	A	93	7.496	16.767	36.226	1.00	33.46
2171	N	ARG	A	94	8.439	12.827	40.06	1.00	38.75
2172	CA	ARG	A	94	8.2	11.496	40.608	1.00	40.44
2173	C	ARG	A	94	8.031	11.6	42.119	1.00	40.42
2174	O	ARG	A	94	7.181	10.931	42.701	1.00	40.21
2175	CB	ARG	A	94	9.356	10.545	40.276	1.00	42.07
2176	CG	ARG	A	94	10.588	10.752	41.134	1.00	45.21
2177	CD	ARG	A	94	11.784	9.955	40.645	1.00	47.2
2178	NE	ARG	A	94	13.005	10.391	41.319	1.00	49.11
2179	CZ	ARG	A	94	14.23	10.02	40.965	1.00	49.97
2180	NH1	ARG	A	94	15.279	10.472	41.641	1.00	50.7
2181	NH2	ARG	A	94	14.405	9.203	39.934	1.00	50.37
2182	N	MET	A	95	8.838	12.447	42.754	1.00	40.55
2183	CA	MET	A	95	8.758	12.623	44.198	1.00	40.86
2184	C	MET	A	95	7.426	13.255	44.593	1.00	41.15
2185	O	MET	A	95	6.82	12.874	45.59	1.00	40.85
2186	CB	MET	A	95	9.913	13.495	44.695	1.00	40.8
2187	CG	MET	A	95	11.281	12.84	44.591	1.00	41.15
2188	SD	MET	A	95	12.618	13.905	45.18	1.00	41.3
2189	CE	MET	A	95	13.504	14.218	43.666	1.00	41.51
2190	N	LEU	A	96	6.974	14.215	43.796	1.00	41.72
2191	CA	LEU	A	96	5.721	14.912	44.054	1.00	43.05
2192	C	LEU	A	96	4.473	14.036	43.916	1.00	44.43
2193	O	LEU	A	96	3.498	14.219	44.65	1.00	44.06
2194	CB	LEU	A	96	5.599	16.116	43.116	1.00	42.37
2195	CG	LEU	A	96	6.444	17.347	43.453	1.00	42.5
2196	CD1	LEU	A	96	6.466	18.306	42.275	1.00	41.75
2197	CD2	LEU	A	96	5.87	18.022	44.688	1.00	42.41
2198	N	GLU	A	97	4.502	13.091	42.981	1.00	45.86
2199	CA	GLU	A	97	3.357	12.214	42.755	1.00	48.09

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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

2200	C	GLU	A	97	3.098	11.216	43.876	1.00	48.66
2201	O	GLU	A	97	2.007	10.656	43.976	1.00	48.83
2202	CB	GLU	A	97	3.52	11.46	41.442	1.00	48.99
2203	CG	GLU	A	97	3.618	12.365	40.243	1.00	51.4
2204	CD	GLU	A	97	3.556	11.6	38.948	1.00	52.67
2205	OE1	GLU	A	97	4.288	10.594	38.82	1.00	54.02
2206	OE2	GLU	A	97	2.775	12.007	38.061	1.00	53.8
2207	N	GLU	A	98	4.097	10.99	44.716	1.00	49.28
2208	CA	GLU	A	98	3.947	10.061	45.82	1.00	50.38
2209	C	GLU	A	98	3.389	10.789	47.039	1.00	50.76
2210	O	GLU	A	98	3.501	12.012	47.149	1.00	51.31
2211	CB	GLU	A	98	5.298	9.436	46.152	1.00	51.2
2212	CG	GLU	A	98	6.092	9.057	44.919	1.00	52.5
2213	CD	GLU	A	98	7.049	7.912	45.164	1.00	53.71
2214	OE1	GLU	A	98	7.941	8.039	46.03	1.00	54.37
2215	OE2	GLU	A	98	6.903	6.875	44.483	1.00	54.87
2216	N	ALA	A	99	2.772	10.043	47.949	1.00	50.95
2217	CA	ALA	A	99	2.215	10.646	49.155	1.00	50.79
2218	C	ALA	A	99	3.376	11.11	50.019	1.00	50.22
2219	O	ALA	A	99	3.361	12.214	50.559	1.00	50.65
2220	CB	ALA	A	99	1.363	9.629	49.913	1.00	51.28
2221	N	LYS	A	100	4.386	10.251	50.121	1.00	49.03
2222	CA	LYS	A	100	5.59	10.514	50.9	1.00	47.99
2223	C	LYS	A	100	5.959	12.001	50.996	1.00	46.69
2224	O	LYS	A	100	5.814	12.757	50.034	1.00	47.01
2225	CB	LYS	A	100	6.755	9.724	50.295	1.00	48.65
2226	CG	LYS	A	100	8.039	9.755	51.103	1.00	49.71
2227	CD	LYS	A	100	9.118	8.91	50.436	1.00	50.6
2228	CE	LYS	A	100	10.427	8.947	51.214	1.00	51.27
2229	NZ	LYS	A	100	11.501	8.164	50.532	1.00	51.98
2230	N	THR	A	101	6.422	12.407	52.174	1.00	44.64
2231	CA	THR	A	101	6.836	13.783	52.435	1.00	42.37
2232	C	THR	A	101	8.361	13.784	52.353	1.00	40.69
2233	O	THR	A	101	9.024	13.109	53.139	1.00	40.49
2234	CB	THR	A	101	6.402	14.23	53.853	1.00	42.75
2235	OG1	THR	A	101	4.979	14.129	53.967	1.00	43.13
2236	CG2	THR	A	101	6.82	15.671	54.126	1.00	43.2
2237	N	TYR	A	102	8.917	14.536	51.409	1.00	38.43
2238	CA	TYR	A	102	10.366	14.568	51.242	1.00	36.39
2239	C	TYR	A	102	11.094	15.617	52.059	1.00	34.44

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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

2240	O	TYR	A	102	12.267	15.452	52.39	1.00	33.83
2241	CB	TYR	A	102	10.711	14.739	49.768	1.00	37.6
2242	CG	TYR	A	102	10.298	13.548	48.953	1.00	38.6
2243	CD1	TYR	A	102	8.957	13.329	48.633	1.00	39.31
2244	CD2	TYR	A	102	11.237	12.607	48.552	1.00	39.02
2245	CE1	TYR	A	102	8.565	12.199	47.935	1.00	40.08
2246	CE2	TYR	A	102	10.858	11.475	47.856	1.00	40.18
2247	CZ	TYR	A	102	9.522	11.275	47.551	1.00	40.29
2248	OH	TYR	A	102	9.152	10.142	46.87	1.00	42
2249	N	VAL	A	103	10.398	16.699	52.373	1.00	32.19
2250	CA	VAL	A	103	10.975	17.774	53.158	1.00	30.5
2251	C	VAL	A	103	10.037	17.976	54.337	1.00	30.05
2252	O	VAL	A	103	8.85	18.246	54.16	1.00	30.43
2253	CB	VAL	A	103	11.072	19.075	52.325	1.00	30.12
2254	CG1	VAL	A	103	11.759	20.17	53.123	1.00	28.95
2255	CG2	VAL	A	103	11.832	18.802	51.038	1.00	29.32
2256	N	ASN	A	104	10.564	17.821	55.542	1.00	29.14
2257	CA	ASN	A	104	9.746	17.977	56.73	1.00	28.34
2258	C	ASN	A	104	9.625	19.432	57.159	1.00	28.17
2259	O	ASN	A	104	10.58	20.194	57.058	1.00	26.68
2260	CB	ASN	A	104	10.321	17.148	57.877	1.00	27.44
2261	CG	ASN	A	104	9.501	17.272	59.146	1.00	27.15
2262	OD1	ASN	A	104	8.277	17.168	59.116	1.00	26.71
2263	ND2	ASN	A	104	10.173	17.484	60.269	1.00	26.7
2264	N	THR	A	105	8.437	19.804	57.628	1.00	28.77
2265	CA	THR	A	105	8.166	21.158	58.101	1.00	29.63
2266	C	THR	A	105	7.341	21.039	59.382	1.00	29.96
2267	O	THR	A	105	6.82	22.026	59.913	1.00	29.81
2268	CB	THR	A	105	7.383	21.993	57.044	1.00	29.47
2269	OG1	THR	A	105	6.069	21.453	56.865	1.00	30.1
2270	CG2	THR	A	105	8.101	21.967	55.712	1.00	28.89
2271	N	THR	A	106	7.248	19.811	59.88	1.00	30.59
2272	CA	THR	A	106	6.492	19.508	61.091	1.00	30.91
2273	C	THR	A	106	7.398	19.428	62.303	1.00	31.18
2274	O	THR	A	106	8.512	18.919	62.22	1.00	31.39
2275	CB	THR	A	106	5.75	18.159	60.952	1.00	31.2
2276	OG1	THR	A	106	4.803	18.25	59.885	1.00	31.22
2277	CG2	THR	A	106	5.018	17.799	62.242	1.00	31.39
2278	N	LEU	A	107	6.919	19.938	63.429	1.00	31.74
2279	CA	LEU	A	107	7.69	19.896	64.659	1.00	32.83



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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

2280	C	LEU	A	107	7.414	18.605	65.395	1.00	34.06
2281	O	LEU	A	107	6.306	18.389	65.879	1.00	34.96
2282	CB	LEU	A	107	7.321	21.053	65.584	1.00	32.01
2283	CG	LEU	A	107	7.921	22.422	65.304	1.00	32.08
2284	CD1	LEU	A	107	7.446	23.398	66.372	1.00	32.05
2285	CD2	LEU	A	107	9.447	22.318	65.298	1.00	31.92
2286	N	TYR	A	108	8.411	17.738	65.466	1.00	35.03
2287	CA	TYR	A	108	8.246	16.5	66.199	1.00	36.35
2288	C	TYR	A	108	8.978	16.687	67.518	1.00	36.56
2289	O	TYR	A	108	8.472	17.366	68.41	1.00	36.96
2290	CB	TYR	A	108	8.803	15.325	65.399	1.00	37.07
2291	CG	TYR	A	108	7.982	15.062	64.164	1.00	38.58
2292	CD1	TYR	A	108	8.467	15.371	62.895	1.00	38.86
2293	CD2	TYR	A	108	6.687	14.552	64.269	1.00	39.04
2294	CE1	TYR	A	108	7.682	15.178	61.759	1.00	39.36
2295	CE2	TYR	A	108	5.895	14.357	63.143	1.00	39.66
2296	CZ	TYR	A	108	6.396	14.671	61.893	1.00	39.7
2297	OH	TYR	A	108	5.606	14.477	60.784	1.00	40.43
2298	N	GLU	A	109	10.171	16.124	67.644	1.00	36.75
2299	CA	GLU	A	109	10.92	16.283	68.882	1.00	37.33
2300	C	GLU	A	109	12.165	17.137	68.686	1.00	36.15
2301	O	GLU	A	109	12.769	17.606	69.652	1.00	36.03
2302	CB	GLU	A	109	11.29	14.913	69.45	1.00	39.8
2303	CG	GLU	A	109	10.061	14.105	69.847	1.00	43.4
2304	CD	GLU	A	109	10.395	12.801	70.539	1.00	45.57
2305	OE1	GLU	A	109	9.447	12.065	70.891	1.00	47.25
2306	OE2	GLU	A	109	11.596	12.511	70.733	1.00	47.03
2307	N	LYS	A	110	12.532	17.356	67.429	1.00	34.5
2308	CA	LYS	A	110	13.704	18.157	67.129	1.00	32.93
2309	C	LYS	A	110	13.636	18.805	65.747	1.00	31.12
2310	O	LYS	A	110	13.123	18.215	64.799	1.00	30.54
2311	CB	LYS	A	110	14.957	17.29	67.238	1.00	33.76
2312	CG	LYS	A	110	16.229	18.102	67.217	1.00	37.02
2313	CD	LYS	A	110	17.472	17.25	67.411	1.00	38.4
2314	CE	LYS	A	110	18.684	18.147	67.534	1.00	38.95
2315	NZ	LYS	A	110	19.97	17.402	67.607	1.00	40.29
2316	N	PHE	A	111	14.139	20.03	65.645	1.00	28.85
2317	CA	PHE	A	111	14.152	20.738	64.372	1.00	27.39
2318	C	PHE	A	111	15.258	21.787	64.401	1.00	26.43
2319	O	PHE	A	111	15.526	22.397	65.436	1.00	26.58

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TABLE 5  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

2320	CB	PHE	A	111	12.786	21.387	64.09	1.00	26.12
2321	CG	PHE	A	111	12.598	21.798	62.653	1.00	25.38
2322	CD1	PHE	A	111	13.087	23.015	62.19	1.00	24.9
2323	CD2	PHE	A	111	12.006	20.929	61.742	1.00	25.14
2324	CE1	PHE	A	111	12.996	23.357	60.837	1.00	24.88
2325	CE2	PHE	A	111	11.91	21.262	60.385	1.00	24.72
2326	CZ	PHE	A	111	12.409	22.478	59.935	1.00	24.55
2327	N	THR	A	112	15.907	21.982	63.261	1.00	25.83
2328	CA	THR	A	112	17.001	22.937	63.153	1.00	25.01
2329	C	THR	A	112	16.81	23.912	61.99	1.00	24.59
2330	O	THR	A	112	16.491	23.503	60.875	1.00	24.43
2331	CB	THR	A	112	18.34	22.195	62.937	1.00	25.43
2332	OG1	THR	A	112	18.559	21.282	64.016	1.00	25.88
2333	CG2	THR	A	112	19.496	23.174	62.868	1.00	25.2
2334	N	TYR	A	113	16.991	25.201	62.255	1.00	23.84
2335	CA	TYR	A	113	16.895	26.202	61.198	1.00	23.35
2336	C	TYR	A	113	18.319	26.51	60.775	1.00	23.73
2337	O	TYR	A	113	19.166	26.791	61.625	1.00	24.16
2338	CB	TYR	A	113	16.262	27.498	61.705	1.00	23.18
2339	CG	TYR	A	113	14.752	27.527	61.732	1.00	23.77
2340	CD1	TYR	A	113	14.082	28.335	62.648	1.00	24.36
2341	CD2	TYR	A	113	13.99	26.773	60.843	1.00	23.42
2342	CE1	TYR	A	113	12.7	28.393	62.686	1.00	24.74
2343	CE2	TYR	A	113	12.589	26.824	60.874	1.00	24.37
2344	CZ	TYR	A	113	11.959	27.638	61.803	1.00	24.43
2345	OH	TYR	A	113	10.594	27.695	61.885	1.00	24.93
2346	N	ALA	A	114	18.589	26.447	59.474	1.00	23.59
2347	CA	ALA	A	114	19.918	26.758	58.962	1.00	23.4
2348	C	ALA	A	114	20.163	28.26	59.15	1.00	24.01
2349	O	ALA	A	114	19.25	29.073	58.993	1.00	22.53
2350	CB	ALA	A	114	20.01	26.383	57.489	1.00	23.11
2351	N	GLY	A	115	21.395	28.629	59.483	1.00	25.1
2352	CA	GLY	A	115	21.705	30.031	59.706	1.00	26.96
2353	C	GLY	A	115	21.591	30.94	58.494	1.00	29.42
2354	O	GLY	A	115	21.74	30.502	57.354	1.00	27.82
2355	N	ILE	A	116	21.32	32.217	58.743	1.00	31.96
2356	CA	ILE	A	116	21.216	33.197	57.67	1.00	35.7
2357	C	ILE	A	116	22.038	34.455	57.986	1.00	38.46
2358	O	ILE	A	116	22.085	35.391	57.192	1.00	38.97
2359	CB	ILE	A	116	19.745	33.596	57.415	1.00	35.07

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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

2360	CG1	ILE	A	116	19.179	34.327	58.634	1.00	35.72
2361	CG2	ILE	A	116	18.916	32.35	57.118	1.00	34.8
2362	CD1	ILE	A	116	17.708	34.689	58.508	1.00	35.3
2363	N	ASP	A	117	22.692	34.465	59.146	1.00	41.74
2364	CA	ASP	A	117	23.521	35.598	59.56	1.00	44.98
2365	C	ASP	A	117	24.925	35.464	58.982	1.00	45.76
2366	O	ASP	A	117	25.243	36.067	57.958	1.00	46.41
2367	CB	ASP	A	117	23.626	35.662	61.084	1.00	47.26
2368	CG	ASP	A	117	22.549	34.855	61.777	1.00	49.57
2369	OD1	ASP	A	117	21.346	35.126	61.543	1.00	50.53
2370	OD2	ASP	A	117	22.912	33.946	62.558	1.00	50.89
2371	N	CYS	A	118	25.758	34.666	59.647	1.00	46.69
2372	CA	CYS	A	118	27.135	34.427	59.219	1.00	48.36
2373	C	CYS	A	118	27.95	35.694	58.952	1.00	48.74
2374	OT1	CYS	A	118	27.484	36.795	59.31	1.00	49.3
2375	CB	CYS	A	118	27.154	33.527	57.975	1.00	49.27
2376	SG	CYS	A	118	25.58	33.388	57.076	1.00	51.64
2377	OT2	CYS	A	118	29.063	35.567	58.399	1.00	49.06
2378	O	HOH		1	4.52	26.361	42.614	1.00	31
2379	O	HOH		2	5.321	22.629	39.881	1.00	23.74
2380	O	HOH		3	2.932	36.52	38.66	1.00	22.55
2381	O	HOH		4	1.712	41.12	35.931	1.00	28.3
2382	O	HOH		5	1.185	36.093	36.748	1.00	50.17
2383	O	HOH		6	-1.455	34.933	44.438	1.00	13.84
2384	O	HOH		7	3.01	37.518	50.131	1.00	34.21
2385	O	HOH		8	6.069	40.644	49.378	1.00	47.59
2386	O	HOH		9	6.852	41.712	44.784	1.00	37.83
2387	O	HOH		10	6.979	41.898	40.893	1.00	27.23
2388	O	HOH		11	13.629	41.28	44.633	1.00	8.78
2389	O	HOH		12	16.162	39.768	44.885	1.00	33.74
2390	O	HOH		13	19.282	39.384	42.467	1.00	40.78
2391	O	HOH		14	21.004	35.625	48.481	1.00	27.51
2392	O	HOH		15	19.534	33.672	47	1.00	18.73
2393	O	HOH		16	20.323	31.931	50.917	1.00	16.79
2394	O	HOH		17	21.78	34.177	50.934	1.00	28.03
2395	O	HOH		18	21.806	38.653	39.833	1.00	37.47
2396	O	HOH		19	24.955	38.295	40.307	1.00	39.39
2397	O	HOH		20	28.053	35.65	38.198	1.00	44.35
2398	O	HOH		21	28.052	36.928	35.949	1.00	39.94
2399	O	HOH		22	21.168	40.116	28.508	1.00	31.15

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TABLE 5  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

2400	O	HOH		23	18.731	41.274	28.711	1.00	38.04
2401	O	HOH		24	17.888	38.518	29.634	1.00	24.04
2402	O	HOH		25	26.181	36.183	26.002	1.00	34.86
2403	O	HOH		26	32.744	35.574	36.784	1.00	33.27
2404	O	HOH		27	16.474	25.409	58.026	1.00	19.3
2405	O	HOH		28	16.692	23.017	57.275	1.00	28.31
2406	O	HOH		29	19.721	21.862	58.954	1.00	26.68
2407	O	HOH		30	16.797	21.193	59.505	1.00	31.38
2408	O	HOH		31	15.42	19.61	61.29	1.00	25.74
2409	O	HOH		32	22.699	28.259	56.501	1.00	25.41
2410	O	HOH		33	17.302	19.025	64.063	1.00	35.17
2411	O	HOH		34	13.327	17.703	60.654	1.00	23.18
2412	O	HOH		35	10.745	18.053	64.011	1.00	37.89
2413	O	HOH		36	11.973	14.868	65.302	1.00	30.39
2414	O	HOH		37	5.987	18.076	57.093	1.00	34.56
2415	O	HOH		38	4.445	19.207	54.802	1.00	26.99
2416	O	HOH		39	3.071	18.183	51.778	1.00	27.78
2417	O	HOH		40	4.051	23.257	57.043	1.00	42.54
2418	O	HOH		41	6.334	15.993	49.394	1.00	30.52
2419	O	HOH		42	5.524	13.968	47.453	1.00	32.05
2420	O	HOH		43	2.725	14.696	50.113	1.00	56.4
2421	O	HOH		44	5.781	19.384	34.73	1.00	19.94
2422	O	HOH		45	15.495	12.096	35.493	1.00	38.21
2423	O	HOH		46	14.861	11.654	32.988	1.00	35.75
2424	O	HOH		47	18.067	15.224	29.07	1.00	37.7
2425	O	HOH		48	17.254	20.274	29.864	1.00	29.82
2426	O	HOH		49	17.445	17.998	28.123	1.00	49.09
2427	O	HOH		50	19.614	21.444	30.682	1.00	33.49
2428	O	HOH		51	23.067	19.934	32.4	1.00	37.3
2429	O	HOH		52	24.106	13.302	32.769	1.00	59.5
2430	O	HOH		53	36.205	15.115	33.303	1.00	67.61
2431	O	HOH		54	32.263	14.166	38.43	1.00	28.58
2432	O	HOH		55	29.878	12.065	39.275	1.00	56.61
2433	O	HOH		56	32.157	15.07	42.015	1.00	36.54
2434	O	HOH		57	30.16	14.581	44.801	1.00	43.51
2435	O	HOH		58	27.813	22.259	47.572	1.00	24.94
2436	O	HOH		59	23.673	11.672	44.322	1.00	35.38
2437	O	HOH		60	16.942	11.647	43.32	1.00	52.24
2438	O	HOH		61	15.944	9.554	54.039	1.00	36.93
2439	O	HOH		62	16.919	14.156	60.706	1.00	44.03

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TABLE 5  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

2440	O	HOH		63	26.531	22.749	55.004	1.00	26.53
2441	O	HOH		64	29.119	24.189	54.681	1.00	39.15
2442	O	HOH		65	29.022	25.814	56.986	1.00	30.42
2443	O	HOH		66	25.79	25.582	55.265	1.00	32.94
2444	O	HOH		67	23.361	30.225	37.8	1.00	34.69
2445	O	HOH		68	28.542	29.312	38.171	1.00	29.23
2446	O	HOH		69	26.15	29.618	35.511	1.00	30.49
2447	O	HOH		70	30.349	24.139	32.705	1.00	23.77
2448	O	HOH		71	32.716	24.682	31.249	1.00	28.69
2449	O	HOH		72	30.104	22.184	30.391	1.00	34.1
2450	O	HOH		73	26.161	23.235	29.115	1.00	37.45
2451	O	HOH		74	25.65	25.576	27.844	1.00	19.22
2452	O	HOH		75	23.365	25.525	26.791	1.00	36.95
2453	O	HOH		76	21.126	24.627	26.09	1.00	43.15
2454	O	HOH		77	22.614	27.902	26.717	1.00	35.32
2455	O	HOH		78	39.085	33.338	36.354	1.00	48.01
2456	O	HOH		79	43.643	29.39	36.04	1.00	56.36
2457	O	HOH		80	35.365	33.708	38.837	1.00	41.53
2458	O	HOH		81	30.482	27.675	45.057	1.00	25.18
2459	O	HOH		82	28.413	26.388	45.67	1.00	20.12
2460	O	HOH		83	27.877	34.778	47.547	1.00	11.31
2461	O	HOH		84	35.407	25.952	29.222	1.00	21.14
2462	O	HOH		85	26.417	24.701	22.41	1.00	45.77
2463	O	HOH		86	1.248	32.636	37.641	1.00	30.36
2464	O	HOH		87	-1.03	31.025	37.535	1.00	31.89
2465	O	HOH		88	12.307	25.943	25.236	1.00	37.9
2466	O	HOH		89	9.343	24.253	27.36	1.00	40.34
2467	O	HOH		90	8.194	23.444	29.774	1.00	35.07
2468	O	HOH		91	0.545	19.448	50.942	1.00	38.92
2469	O	HOH		92	0.691	19.232	53.75	1.00	51.63
2470	O	HOH		93	3.808	32.408	54.559	1.00	42.37
2471	O	HOH		94	6.115	33.316	53.712	1.00	22.03
2472	O	HOH		95	6.186	32.435	60.145	1.00	25.59
2473	O	HOH		96	4.537	34.79	62.739	1.00	26.05
2474	O	HOH		97	8.77	37.618	49.61	1.00	40.06
2475	O	HOH		98	8.464	37.603	27.54	1.00	34.97
2476	O	HOH		99	10.448	38.038	25.066	1.00	39.93
2477	O	HOH		100	2.555	37.001	32.261	1.00	37.16
2478	O	HOH		101	3.293	31.981	29.87	1.00	14.38
2479	O	HOH		102	5.152	33.722	33.679	1.00	29.24

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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

2480	O	HOH		103	3.853	26.659	36.74	1.00	23.23
2481	O	HOH		104	3.576	24.845	34.232	1.00	30.1
2482	O	HOH		105	4.498	24.907	31.321	1.00	41.41
2483	O	HOH		106	-2.923	41.264	36.973	1.00	55.31
2484	O	HOH		107	15.024	55.073	36.163	1.00	52.79
2485	O	HOH		108	0.405	54.544	44.381	1.00	50.06
2486	O	HOH		109	10.528	44.944	47.035	1.00	28.63
2487	O	HOH		110	21.532	37.358	37.06	1.00	33.9
2488	O	HOH		111	16.709	45.727	43.855	1.00	33.96
2489	O	HOH		112	17.95	49.15	40.388	1.00	35.73
2490	O	HOH		113	0.346	46.388	40.609	1.00	45.82
2491	O	HOH		114	0.433	57.044	37.135	1.00	32.26
2492	O	HOH		115	13.171	50.838	36.746	1.00	38.21
2493	O	HOH		116	23.895	27.464	60.384	1.00	36.23
2494	O	HOH		117	25.161	25.726	59.497	1.00	41.62
2495	O	HOH		118	24.203	26.105	57.182	1.00	40.93
2496	O	HOH		119	4.78	20.867	69.151	1.00	43.51
2497	O	HOH		120	4.059	22.716	59.391	1.00	30.45
2498	O	HOH		121	7.691	14.197	34.487	1.00	37.95
2499	O	HOH		122	11.606	16.761	31.842	1.00	36.5
2500	O	HOH		123	14.45	13.45	31.22	1.00	42.88
2501	O	HOH		124	16.345	13.473	29.246	1.00	42.13
2502	O	HOH		125	22.865	17.234	30.088	1.00	36.44
2503	O	HOH		126	25.866	15.848	29.705	1.00	58.08
2504	O	HOH		127	25.59	17.668	31.968	1.00	37.34
2505	O	HOH		128	24.486	20.922	28.847	1.00	46.24
2506	O	HOH		129	32.085	19.86	30.459	1.00	43.37
2507	O	HOH		130	34.272	21.689	37.527	1.00	46.7
2508	O	HOH		131	34.468	15.337	43.642	1.00	54.11
2509	O	HOH		132	35.168	18.523	43.654	1.00	43.74
2510	O	HOH		133	27.981	16.311	44.395	1.00	45.57
2511	O	HOH		134	25.29	15.296	54.649	1.00	37.13
2512	O	HOH		135	35.986	17.04	51.792	1.00	50.85
2513	O	HOH		136	36.951	19.371	52.385	1.00	42.13
2514	O	HOH		137	37.875	34.973	52.787	1.00	41.35
2515	O	HOH		138	34.671	28.361	59.395	1.00	45.92
2516	O	HOH		139	21.433	36.585	53.19	1.00	37.01
2517	O	HOH		140	21.97	37.925	55.42	1.00	50.54
2518	O	HOH		141	26.139	30.262	38.249	1.00	41.66
2519	O	HOH		142	21.07	27.58	30.951	1.00	32.98

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TABLE 5  
STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

2520	O	HOH		143	30.028	23.472	27.537	1.00	46.32
2521	O	HOH		144	35.315	24.583	31.94	1.00	30.46
2522	O	HOH		145	36.621	22.84	33.672	1.00	45.58
2523	O	HOH		146	11.4	50.153	46.783	1.00	40.64
2524	O	HOH		147	15.803	43.286	43.444	1.00	28.17
2525	O	HOH		148	1.571	46.428	19.306	1.00	46.73
2526	O	HOH		149	8.957	41.747	43.015	1.00	40.27
2527	O	HOH		150	21.638	39.269	35.442	1.00	41.41
2528	O	HOH		151	13.365	53.148	38.314	1.00	48.58
2529	O	HOH		152	-6.276	50.604	37.681	1.00	47.99
2530	O	HOH		153	0.612	39.709	38.378	1.00	42.59
2531	O	HOH		154	16.492	50.501	36.026	1.00	50.82
2532	O	HOH		155	19.465	48.021	35.228	1.00	37.85
2533	O	HOH		156	5.553	63.238	25.777	1.00	33.35
2534	O	HOH		157	7.694	60.839	24.31	1.00	43.3
2535	O	HOH		158	16.004	33.481	18.553	1.00	42.58
2536	O	HOH		159	6.499	28.194	26.989	1.00	40.08
2537	O	HOH		160	2.366	26.335	29.526	1.00	48.41
2538	O	HOH		161	2.361	32.93	33.02	1.00	37.57
2539	O	HOH		162	1.695	31.188	35.276	1.00	41.93
2540	O	HOH		163	10.811	59.777	31.061	1.00	43.24
2541	O	HOH		164	9.089	37.34	52.128	1.00	47.85
2542	O	HOH		165	5.855	36.064	53.338	1.00	39.68
2543	O	HOH		166	10.989	40.038	48.479	1.00	50.5
2544	O	HOH		167	13.371	38.216	54.608	1.00	35.15
2545	O	HOH		168	16.468	39.731	50.979	1.00	51.19
2546	O	HOH		169	19.727	38.425	49.145	1.00	29.7
2547	O	HOH		170	20.003	38.548	51.693	1.00	36.33
2548	O	HOH		171	23.839	25.669	24.421	1.00	36.46
2549	O	HOH		172	37.056	23.021	36.704	1.00	48.58
2550	O	HOH		173	25.465	36.428	46.013	1.00	29.38
2551	O	HOH		174	26.824	38.454	45.273	1.00	43.29
2552	O	HOH		175	18.003	13.756	37.82	1.00	48.56
2553	O	HOH		176	22.414	12.377	34.58	1.00	49.97
2554	O	HOH		177	3.705	40.308	25.694	1.00	47.63
2555	O	HOH		178	4.291	53.824	22.639	1.00	46.19
2556	O	HOH		179	3.204	56.813	24.491	1.00	44.15
2557	O	HOH		180	-0.39	57.827	25.421	1.00	41.63
2558	O	HOH		181	1.938	49.487	46.754	1.00	44.12
2559	O	HOH		182	0.008	49.46	45.452	1.00	46.18

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TABLE 5

## STRUCTURE COORDINATES FOR TIE2K CRYSTAL FORM IV

2560	O	HOH		183	4.042	47.281	46.867	1.00	38.93
2561	O	HOH		184	4.546	44.691	45.893	1.00	42.81
2562	O	HOH		185	16.523	49.154	38.052	1.00	43
2563	O	HOH		186	15.511	52.423	36.945	1.00	59.95
2564	O	HOH		187	-4.752	44.531	29.723	1.00	47.62
2565	O	HOH		188	7.223	31.201	24.021	1.00	46.88
2566	O	HOH		189	1.573	27.828	36.033	1.00	31.72
2567	O	HOH		190	3.308	25.208	38.909	1.00	35.64
2568	O	HOH		191	0.848	26.257	34.161	1.00	47.11
2569	O	HOH		192	1.513	34.44	51.904	1.00	40.95
2570	O	HOH		193	-2.279	35.108	47.41	1.00	33.99
2571	O	HOH		194	10.634	37.534	59.495	1.00	31.46
2572	O	HOH		195	6.648	36.382	58.512	1.00	26.64
2573	O	HOH		196	3.75	33.386	59.77	1.00	36.53
2574	O	HOH		197	4.951	37.374	55.351	1.00	43.53
2575	O	HOH		198	5.483	33.391	70.366	1.00	27.79
2576	O	HOH		199	2.184	33.496	63.567	1.00	38.9
2577	O	HOH		200	1.335	31.874	61.144	1.00	44



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TABLE 6

FGFR1 COORDINATE DATA FOR RESIDUES 464-485

ATOM	ATOM TYPE	RESIDUE	PROTEIN #	#	X	Y	Z	OCC	B
1	C	GLU	A	464	-11.959	15.705	7.33	1.00	50.39
2	CA	GLU	A	464	-12.513	17.08	7.7	1.00	53.29
3	CB	GLU	A	464	-11.398	17.993	8.222	1.00	55.23
4	N	GLU	A	464	-13.594	16.979	8.673	1.00	55.29
5	O	GLU	A	464	-11.971	15.338	6.157	1.00	52.71
6	C	LEU	A	465	-12.067	12.607	7.662	1.00	39.98
7	CA	LEU	A	465	-10.982	13.598	8.042	1.00	41.92
8	CB	LEU	A	465	-10.214	13.056	9.244	1.00	40.83
9	CD1	LEU	A	465	-8.306	14.612	8.848	1.00	47.36
10	CD2	LEU	A	465	-8.04	12.664	10.397	1.00	41.14
11	CG	LEU	A	465	-8.698	13.166	9.126	1.00	43.96
12	N	LEU	A	465	-11.519	14.929	8.316	1.00	45.67
13	O	LEU	A	465	-13.163	12.626	8.219	1.00	39.16
14	C	PRO	A	466	-12.884	9.607	7.236	1.00	35.95
15	CA	PRO	A	466	-12.746	10.733	6.222	1.00	36.69
16	CB	PRO	A	466	-12.127	10.247	4.914	1.00	38.01
17	CD	PRO	A	466	-10.566	11.74	5.844	1.00	37.53
18	CG	PRO	A	466	-10.64	10.398	5.173	1.00	37.05
19	N	PRO	A	466	-11.781	11.744	6.675	1.00	38.02
20	O	PRO	A	466	-11.904	9.185	7.847	1.00	35.07
21	C	GLU	A	467	-13.892	6.733	7.806	1.00	32.54
22	CA	GLU	A	467	-14.344	8.06	8.386	1.00	35.33
23	CB	GLU	A	467	-15.836	7.981	8.711	1.00	41.21
24	CD	GLU	A	467	-17.88	9.181	9.64	1.00	50.36
25	CG	GLU	A	467	-16.468	9.312	9.071	1.00	48.72
26	N	GLU	A	467	-14.106	9.126	7.43	1.00	35.56
27	O	GLU	A	467	-13.985	6.528	6.597	1.00	34.84
28	OE1	GLU	A	467	-18.416	8.057	9.669	1.00	52.62
29	OE2	GLU	A	467	-18.437	10.208	10.068	1.00	51.73
30	C	ASP	A	468	-13.283	3.581	9.377	1.00	29.51
31	CA	ASP	A	468	-12.912	4.535	8.259	1.00	28.78
32	CB	ASP	A	468	-11.41	4.443	7.993	1.00	29.14
33	CG	ASP	A	468	-11.002	3.086	7.425	1.00	27.31
34	N	ASP	A	468	-13.339	5.871	8.656	1.00	30.54
35	O	ASP	A	468	-12.509	3.367	10.323	1.00	27.71
36	OD1	ASP	A	468	-11.842	2.162	7.365	1.00	27.24
37	OD2	ASP	A	468	-9.833	2.938	7.028	1.00	31
38	C	PRO	A	469	-14.02	0.851	10.551	1.00	28.91
39	CA	PRO	A	469	-14.983	1.99	10.227	1.00	30.22

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TABLE 6

FGFR1 COORDINATE DATA FOR RESIDUES 464-485

40	CB	PRO	A	469	-16.252	1.464	9.537	1.00	33.81
41	CD	PRO	A	469	-15.381	3.085	8.104	1.00	28.92
42	CG	PRO	A	469	-16.685	2.618	8.679	1.00	31.27
43	N	PRO	A	469	-14.456	2.942	9.247	1.00	29.55
44	O	PRO	A	469	-14.109	0.245	11.618	1.00	28.31
45	C	ARG	A	470	-11.189	-0.275	10.978	1.00	29.33
46	CA	ARG	A	470	-12.142	-0.512	9.807	1.00	27.2
47	CB	ARG	A	470	-11.303	-0.699	8.532	1.00	28.12
48	CD	ARG	A	470	-11.127	-1.377	6.083	1.00	25.81
49	CG	ARG	A	470	-12.039	-1.304	7.324	1.00	29.47
50	CZ	ARG	A	470	-9.626	0.146	4.822	1.00	32
51	N	ARG	A	470	-13.107	0.563	9.626	1.00	27.62
52	NE	ARG	A	470	-10.498	-0.087	5.802	1.00	30.59
53	NH1	ARG	A	470	-9.258	-0.827	3.992	1.00	32.56
54	NH2	ARG	A	470	-9.105	1.361	4.685	1.00	28.91
55	O	ARG	A	470	-10.774	-1.216	11.646	1.00	29.1
56	C	TRP	A	471	-10.379	2.227	13.436	1.00	28.4
57	CA	TRP	A	471	-9.953	1.32	12.304	1.00	28.54
58	CB	TRP	A	471	-8.739	1.948	11.614	1.00	25.7
59	CD1	TRP	A	471	-8.161	0.859	9.389	1.00	27.7
60	CD2	TRP	A	471	-7.161	-0.051	11.169	1.00	28.15
61	CE2	TRP	A	471	-6.775	-0.776	10.025	1.00	30
62	CE3	TRP	A	471	-6.654	-0.45	12.421	1.00	26.54
63	CG	TRP	A	471	-8.047	0.98	10.746	1.00	25.13
64	CH2	TRP	A	471	-5.426	-2.227	11.311	1.00	28.07
65	CZ2	TRP	A	471	-5.905	-1.863	10.077	1.00	28.96
66	CZ3	TRP	A	471	-5.791	-1.53	12.478	1.00	27.52
67	N	TRP	A	471	-10.92	0.988	11.277	1.00	28.04
68	NE1	TRP	A	471	-7.406	-0.196	8.944	1.00	30.65
69	O	TRP	A	471	-9.657	2.338	14.426	1.00	26.65
70	C	GLU	A	472	-12.225	3.278	15.701	1.00	24.73
71	CA	GLU	A	472	-11.991	3.828	14.298	1.00	26.79
72	CB	GLU	A	472	-13.255	4.54	13.808	1.00	28.13
73	CD	GLU	A	472	-12.701	7.059	14.08	1.00	26.4
74	CG	GLU	A	472	-13.565	5.876	14.537	1.00	28.97
75	N	GLU	A	472	-11.531	2.875	13.294	1.00	28.45
76	O	GLU	A	472	-12.784	2.211	15.864	1.00	25.78
77	OE1	GLU	A	472	-12.145	7.039	12.96	1.00	28.89
78	OE2	GLU	A	472	-12.61	8.043	14.832	1.00	27.71
79	C	LEU	A	473	-12.558	4.862	18.727	1.00	26.64

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TABLE 6

FGFR1 COORDINATE DATA FOR RESIDUES 464-485

80	CA	LEU	A	473	-11.968	3.614	18.097	1.00	26.33
81	CB	LEU	A	473	-10.652	3.269	18.813	1.00	27.73
82	CD1	LEU	A	473	-11.345	1.64	20.616	1.00	24.66
83	CD2	LEU	A	473	-9.384	3.118	20.995	1.00	26.18
84	CG	LEU	A	473	-10.748	3.013	20.33	1.00	26.48
85	N	LEU	A	473	-11.753	3.999	16.708	1.00	24.5
86	O	LEU	A	473	-12.151	5.98	18.38	1.00	25.52
87	C	PRO	A	474	-13.176	6.531	21.12	1.00	30.13
88	CA	PRO	A	474	-14.218	5.878	20.2	1.00	29.38
89	CB	PRO	A	474	-15.37	5.26	21	1.00	28.51
90	CD	PRO	A	474	-14.432	3.505	19.789	1.00	29.97
91	CG	PRO	A	474	-15.768	4.106	20.158	1.00	28.76
92	N	PRO	A	474	-13.613	4.705	19.553	1.00	28.78
93	O	PRO	A	474	-12.439	5.84	21.829	1.00	31.99
94	C	ARG	A	475	-12.202	8.265	23.376	1.00	36.42
95	CA	ARG	A	475	-12.153	8.593	21.904	1.00	33.15
96	CB	ARG	A	475	-12.357	10.091	21.737	1.00	32.69
97	CD	ARG	A	475	-12.083	12.031	20.195	1.00	37.12
98	CG	ARG	A	475	-12.221	10.539	20.327	1.00	37.72
99	CZ	ARG	A	475	-10.541	12.51	18.339	1.00	37.96
100	N	ARG	A	475	-13.109	7.854	21.096	1.00	31.55
101	NE	ARG	A	475	-11.768	12.328	18.805	1.00	40.06
102	NH1	ARG	A	475	-9.503	12.452	19.169	1.00	35.79
103	NH2	ARG	A	475	-10.352	12.676	17.036	1.00	34.32
104	O	ARG	A	475	-11.176	8.303	24.058	1.00	37.7
105	C	ASP	A	476	-12.952	6.298	25.696	1.00	35.51
106	CA	ASP	A	476	-13.532	7.65	25.294	1.00	36.84
107	CB	ASP	A	476	-14.996	7.774	25.732	1.00	37.68
108	CG	ASP	A	476	-15.897	6.749	25.089	1.00	38.79
109	N	ASP	A	476	-13.391	7.958	23.878	1.00	36.94
110	O	ASP	A	476	-12.948	5.939	26.874	1.00	37.54
111	OD1	ASP	A	476	-15.435	5.926	24.28	1.00	43.46
112	OD2	ASP	A	476	-17.098	6.766	25.406	1.00	44.6
113	C	ARG	A	477	-10.585	4.361	25.119	1.00	31.06
114	CA	ARG	A	477	-11.901	4.239	24.975	1.00	31.71
115	CB	ARG	A	477	-12.222	3.264	23.841	1.00	31.61
116	CD	ARG	A	477	-14.36	2.392	24.851	1.00	34.33
117	CG	ARG	A	477	-13.699	2.977	23.615	1.00	30.04
118	CZ	ARG	A	477	-14.857	3.149	27.145	1.00	33.82
119	N	ARG	A	477	-12.492	5.537	24.712	1.00	32.96

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TABLE 6

FGFR1 COORDINATE DATA FOR RESIDUES 464-485

120	NE	ARG	A	477	-14.584	3.408	25.872	1.00	33.93
121	NH1	ARG	A	477	-14.948	1.899	27.577	1.00	30.93
122	NH2	ARG	A	477	-15.026	4.154	27.986	1.00	33.36
123	O	ARG	A	477	-9.697	3.385	25.402	1.00	32.03
124	C	LEU	A	478	-8.045	6.644	26.222	1.00	37.67
125	CA	LEU	A	478	-8.434	5.76	25.035	1.00	35.62
126	CB	LEU	A	478	-7.963	6.391	23.724	1.00	34.62
127	CD1	LEU	A	478	-6.063	4.846	23.212	1.00	29.28
128	CD2	LEU	A	478	-6.307	7.067	22.029	1.00	32.95
129	CG	LEU	A	478	-6.492	6.31	23.34	1.00	35.66
130	N	LEU	A	478	-9.864	5.563	24.959	1.00	32.47
131	O	LEU	A	478	-8.273	7.854	26.208	1.00	41.41
132	C	VAL	A	479	-5.569	7.211	28.201	1.00	35.71
133	CA	VAL	A	479	-7.011	6.748	28.44	1.00	35.71
134	CB	VAL	A	479	-7.075	5.838	29.686	1.00	36.02
135	CG1	VAL	A	479	-6.77	6.64	30.925	1.00	39.35
136	CG2	VAL	A	479	-8.449	5.189	29.808	1.00	34.47
137	N	VAL	A	479	-7.458	6.034	27.247	1.00	36.37
138	O	VAL	A	479	-4.621	6.423	28.305	1.00	33.02
139	C	LEU	A	480	-3.196	9.226	28.788	1.00	45.77
140	CA	LEU	A	480	-4.099	9.059	27.571	1.00	43.66
141	CB	LEU	A	480	-4.249	10.384	26.821	1.00	43.53
142	CD1	LEU	A	480	-5.161	11.744	24.942	1.00	44.49
143	CD2	LEU	A	480	-4.309	9.439	24.488	1.00	45.08
144	CG	LEU	A	480	-5.017	10.337	25.492	1.00	44.08
145	N	LEU	A	480	-5.414	8.488	27.871	1.00	38.5
146	O	LEU	A	480	-3.618	9.768	29.811	1.00	46.1
147	C	GLY	A	481	0.305	9.596	29.526	1.00	51.54
148	CA	GLY	A	481	-1.011	8.873	29.756	1.00	50.08
149	N	GLY	A	481	-1.945	8.794	28.651	1.00	47.08
150	O	GLY	A	481	0.369	10.63	28.859	1.00	52.33
151	C	LYS	A	482	3.304	9.741	28.63	1.00	57.22
152	CA	LYS	A	482	2.707	9.594	30.028	1.00	56.21
153	CB	LYS	A	482	3.646	8.754	30.894	1.00	57.08
154	CD	LYS	A	482	5.954	7.832	31.138	1.00	63.04
155	CE	LYS	A	482	5.542	6.549	30.418	1.00	62.54
156	CG	LYS	A	482	5.121	9.017	30.677	1.00	60.82
157	N	LYS	A	482	1.361	9.032	30.099	1.00	53.24
158	NZ	LYS	A	482	6.313	5.368	30.9	1.00	63.37
159	O	LYS	A	482	3.297	8.799	27.832	1.00	56.52

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TABLE 6

FGFR1 COORDINATE DATA FOR RESIDUES 464-485

160	C	PRO	A	483	5.649	10.242	26.818	1.00	61.76
161	CA	PRO	A	483	4.47	11.195	27.024	1.00	59.93
162	CB	PRO	A	483	4.955	12.636	27.176	1.00	59.19
163	CD	PRO	A	483	3.874	12.134	29.173	1.00	57.57
164	CG	PRO	A	483	3.976	13.223	28.151	1.00	58.78
165	N	PRO	A	483	3.855	10.926	28.327	1.00	58.91
166	O	PRO	A	483	6.485	10.085	27.709	1.00	61.89
167	C	LEU	A	484	7.88	9.28	24.547	1.00	71.47
168	CA	LEU	A	484	6.759	8.636	25.354	1.00	68.45
169	CB	LEU	A	484	6.215	7.429	24.593	1.00	68.64
170	CD1	LEU	A	484	4.737	5.431	24.419	1.00	66.96
171	CD2	LEU	A	484	6.01	5.869	26.554	1.00	68.75
172	CG	LEU	A	484	5.278	6.496	25.363	1.00	69.82
173	N	LEU	A	484	5.683	9.574	25.671	1.00	65.08
174	O	LEU	A	484	9.048	8.925	24.707	1.00	72.44
175	C	GLY	A	485	7.883	11.601	21.674	1.00	76.22
176	CA	GLY	A	485	8.514	10.884	22.85	1.00	75.53
177	N	GLY	A	485	7.521	10.214	23.671	1.00	73.94
178	O	GLY	A	485	6.706	11.963	21.73	1.00	76.68

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TABLE 7

FGFR1 COORDINATE DATA FOR RESIDUES 491-500

ATOM	ATOM TYPE	RESIDUE	PROTEIN #	#	X	Y	Z	OCC	B
179	C	GLN	A	491	3.495	12.46	20.069	1.00	46.45
180	CA	GLN	A	491	4.057	13.882	19.947	1.00	47.03
181	CB	GLN	A	491	3.038	14.897	20.483	1.00	46.35
182	N	GLN	A	491	4.422	14.211	18.572	1.00	50.15
183	O	GLN	A	491	2.564	12.083	19.348	1.00	45.34
184	C	VAL	A	492	3.467	10.112	22.688	1.00	43.96
185	CA	VAL	A	492	3.663	10.294	21.191	1.00	43.47
186	CB	VAL	A	492	4.689	9.249	20.722	1.00	41.45
187	CG1	VAL	A	492	4.128	7.858	20.941	1.00	40.56
188	CG2	VAL	A	492	5.028	9.451	19.26	1.00	42
189	N	VAL	A	492	4.101	11.664	20.947	1.00	45.04
190	O	VAL	A	492	4.326	10.495	23.489	1.00	43.72
191	C	VAL	A	493	1.635	7.887	24.7	1.00	40.11
192	CA	VAL	A	493	2.04	9.328	24.473	1.00	40.83
193	CB	VAL	A	493	0.891	10.246	25	1.00	40.49
194	CG1	VAL	A	493	1.197	11.698	24.727	1.00	42.47
195	CG2	VAL	A	493	-0.447	9.859	24.391	1.00	43.59
196	N	VAL	A	493	2.327	9.55	23.067	1.00	42.35
197	O	VAL	A	493	1.139	7.224	23.788	1.00	40.01
198	C	LEU	A	494	0.078	6.237	26.647	1.00	33.18
199	CA	LEU	A	494	1.535	6.041	26.252	1.00	34.59
200	CB	LEU	A	494	2.356	5.546	27.443	1.00	35.18
201	CD1	LEU	A	494	2.126	3.072	26.965	1.00	36.63
202	CD2	LEU	A	494	2.983	3.883	29.163	1.00	41.76
203	CG	LEU	A	494	2.03	4.168	28.019	1.00	36.71
204	N	LEU	A	494	1.928	7.382	25.89	1.00	36.62
205	O	LEU	A	494	-0.311	7.32	27.092	1.00	32.49
206	C	ALA	A	495	-2.657	3.893	27.035	1.00	30.09
207	CA	ALA	A	495	-2.147	5.291	26.774	1.00	30.94
208	CB	ALA	A	495	-2.936	5.937	25.642	1.00	31.3
209	N	ALA	A	495	-0.739	5.219	26.427	1.00	33.03
210	O	ALA	A	495	-1.934	2.91	26.861	1.00	27.84
211	C	GLU	A	496	-5.812	2.517	26.932	1.00	32.27
212	CA	GLU	A	496	-4.534	2.534	27.75	1.00	31.34
213	CB	GLU	A	496	-4.844	2.394	29.232	1.00	32.57
214	CD	GLU	A	496	-3.887	2.401	31.564	1.00	40.03
215	CG	GLU	A	496	-3.602	2.192	30.092	1.00	37.08
216	N	GLU	A	496	-3.901	3.812	27.482	1.00	30.33
217	O	GLU	A	496	-6.597	3.468	26.974	1.00	33.91

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TABLE 7

FGFR1 COORDINATE DATA FOR RESIDUES 491-500

218	OE1	GLU	A	496	-4.263	3.531	31.931	1.00	40.14
219	OE2	GLU	A	496	-3.751	1.441	32.351	1.00	42.74
220	C	ALA	A	497	-8.061	0.34	25.902	1.00	32.19
221	CA	ALA	A	497	-7.126	1.352	25.255	1.00	32.2
222	CB	ALA	A	497	-6.717	0.881	23.874	1.00	29.44
223	N	ALA	A	497	-5.953	1.496	26.098	1.00	30.62
224	O	ALA	A	497	-7.649	-0.776	26.206	1.00	33.62
225	C	ILE	A	498	-11.007	-0.826	25.626	1.00	35.95
226	CA	ILE	A	498	-10.287	-0.131	26.773	1.00	33.95
227	CB	ILE	A	498	-11.344	0.671	27.594	1.00	34.48
228	CD1	ILE	A	498	-11.556	2.626	29.201	1.00	32.04
229	CG1	ILE	A	498	-10.669	1.515	28.68	1.00	33.93
230	CG2	ILE	A	498	-12.359	-0.283	28.24	1.00	34.04
231	N	ILE	A	498	-9.296	0.75	26.166	1.00	32.8
232	O	ILE	A	498	-11.643	-0.171	24.799	1.00	35.62
233	C	GLY	A	499	-10.682	-3.185	23.283	1.00	53.38
234	CA	GLY	A	499	-11.548	-2.872	24.493	1.00	47.86
235	N	GLY	A	499	-10.878	-2.14	25.546	1.00	40.37
236	O	GLY	A	499	-9.973	-4.199	23.271	1.00	55.85
237	C	LEU	A	500	-10.504	-3.692	20.254	1.00	56.6
238	CA	LEU	A	500	-9.977	-2.485	21.032	1.00	56.41
239	CB	LEU	A	500	-8.463	-2.644	21.271	1.00	56.56
240	CD1	LEU	A	500	-6.107	-1.881	21.349	1.00	54.46
241	CD2	LEU	A	500	-7.713	-0.646	19.914	1.00	52.37
242	CG	LEU	A	500	-7.544	-1.418	21.216	1.00	55.46
243	N	LEU	A	500	-10.721	-2.304	22.284	1.00	54.89
244	O	LEU	A	500	-10.334	-4.844	20.667	1.00	57.46

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TABLE 8

FGFR1 COORDINATE DATA FOR RESIDUES 506-578

ATOM	ATOM TYPE	RESIDUE	PROTEIN #	#	X	Y	Z	OCC	B
252	C	ASN	A	506	-11.939	-5.011	29.932	1.00	45.13
253	CA	ASN	A	506	-13.423	-4.891	29.577	1.00	45.16
254	CB	ASN	A	506	-14.261	-5.727	30.55	1.00	45.69
255	CG	ASN	A	506	-15.734	-5.409	30.464	1.00	46.02
256	N	ASN	A	506	-13.727	-5.252	28.197	1.00	43.05
257	ND2	ASN	A	506	-16.555	-6.441	30.378	1.00	49.28
258	O	ASN	A	506	-11.57	-5.082	31.111	1.00	44.81
259	OD1	ASN	A	506	-16.129	-4.249	30.464	1.00	47.66
260	C	ARG	A	507	-8.963	-3.903	28.54	1.00	40.31
261	CA	ARG	A	507	-9.653	-5.134	29.096	1.00	45.15
262	CB	ARG	A	507	-9.128	-6.358	28.338	1.00	53.01
263	CD	ARG	A	507	-8.32	-8.031	30.027	1.00	67.96
264	CG	ARG	A	507	-9.392	-7.697	29.002	1.00	61.48
265	CZ	ARG	A	507	-7.979	-9.82	31.701	1.00	80.06
266	N	ARG	A	507	-11.093	-5.016	28.911	1.00	45.54
267	NE	ARG	A	507	-8.506	-9.378	30.562	1.00	74.91
268	NH1	ARG	A	507	-7.211	-9.029	32.446	1.00	79.99
269	NH2	ARG	A	507	-8.277	-11.041	32.129	1.00	83.31
270	O	ARG	A	507	-9.377	-3.376	27.51	1.00	36.25
271	C	VAL	A	508	-5.896	-2.81	28.168	1.00	34.49
272	CA	VAL	A	508	-7.189	-2.272	28.769	1.00	36.93
273	CB	VAL	A	508	-6.849	-1.234	29.887	1.00	35.89
274	CG1	VAL	A	508	-8.121	-0.736	30.543	1.00	39.86
275	CG2	VAL	A	508	-5.909	-1.815	30.914	1.00	36.28
276	N	VAL	A	508	-7.947	-3.419	29.246	1.00	38.92
277	O	VAL	A	508	-5.384	-3.846	28.605	1.00	33.11
278	C	THR	A	509	-3.269	-1.296	26.468	1.00	28.32
279	CA	THR	A	509	-4.169	-2.519	26.488	1.00	31.71
280	CB	THR	A	509	-4.435	-2.944	25.011	1.00	33.96
281	CG2	THR	A	509	-3.158	-3.449	24.34	1.00	30.94
282	N	THR	A	509	-5.408	-2.134	27.139	1.00	30.46
283	O	THR	A	509	-3.725	-0.217	26.126	1.00	27.97
284	OG1	THR	A	509	-5.425	-3.979	24.979	1.00	40.32
285	C	LYS	A	510	-0.757	-0.157	25.375	1.00	28.44
286	CA	LYS	A	510	-1.104	-0.3	26.847	1.00	30.27
287	CB	LYS	A	510	0.171	-0.549	27.644	1.00	27.93
288	CD	LYS	A	510	1.31	-0.69	29.836	1.00	40.64
289	CE	LYS	A	510	1.157	-1.629	31.035	1.00	46.31
290	CG	LYS	A	510	-0.013	-0.478	29.127	1.00	34.3



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TABLE 8  
FGFR1 COORDINATE DATA FOR RESIDUES 506-578

291	N	LYS	A	510	-2.023	-1.433	26.911	1.00	29.33
292	NZ	LYS	A	510	0.41	-1.027	32.187	1.00	49.1
293	O	LYS	A	510	-0.393	-1.136	24.723	1.00	28.66
294	C	VAL	A	511	0.137	2.668	23.361	1.00	29.35
295	CA	VAL	A	511	-0.626	1.347	23.467	1.00	29.42
296	CB	VAL	A	511	-1.95	1.46	22.652	1.00	26.93
297	CG1	VAL	A	511	-2.688	0.112	22.639	1.00	24.68
298	CG2	VAL	A	511	-2.842	2.575	23.226	1.00	21.96
299	N	VAL	A	511	-0.904	1.055	24.86	1.00	28.85
300	O	VAL	A	511	0.25	3.404	24.342	1.00	33.12
301	C	ALA	A	512	0.498	5.016	21.06	1.00	25.39
302	CA	ALA	A	512	1.409	4.196	21.96	1.00	25.7
303	CB	ALA	A	512	2.748	3.95	21.28	1.00	24.81
304	N	ALA	A	512	0.703	2.94	22.188	1.00	27.76
305	O	ALA	A	512	-0.066	4.489	20.115	1.00	27.73
306	C	VAL	A	513	0.242	8.338	19.929	1.00	34.25
307	CA	VAL	A	513	-0.519	7.17	20.572	1.00	32.1
308	CB	VAL	A	513	-1.709	7.722	21.421	1.00	32.09
309	CG1	VAL	A	513	-2.602	8.609	20.57	1.00	32.35
310	CG2	VAL	A	513	-2.528	6.57	22.014	1.00	31.72
311	N	VAL	A	513	0.341	6.297	21.359	1.00	28.84
312	O	VAL	A	513	0.802	9.192	20.622	1.00	34.2
313	C	LYS	A	514	-0.112	10.491	17.473	1.00	36.47
314	CA	LYS	A	514	0.879	9.396	17.796	1.00	36.23
315	CB	LYS	A	514	1.381	8.803	16.487	1.00	36.5
316	CD	LYS	A	514	2.565	6.947	15.315	1.00	45.97
317	CE	LYS	A	514	3.892	7.628	14.988	1.00	49.81
318	CG	LYS	A	514	1.998	7.436	16.632	1.00	40.25
319	N	LYS	A	514	0.221	8.366	18.596	1.00	36.47
320	NZ	LYS	A	514	3.801	9.071	14.61	1.00	53.65
321	O	LYS	A	514	-1.229	10.218	17.016	1.00	34.96
322	C	MET	A	515	0.316	14.064	17.014	1.00	44.67
323	CA	MET	A	515	-0.545	12.879	17.427	1.00	42
324	CB	MET	A	515	-1.373	13.242	18.658	1.00	42.88
325	CE	MET	A	515	-1.665	12.068	21.893	1.00	44.43
326	CG	MET	A	515	-0.531	13.582	19.864	1.00	45.26
327	N	MET	A	515	0.3	11.731	17.697	1.00	38.07
328	O	MET	A	515	1.548	14.009	17.078	1.00	45.57
329	SD	MET	A	515	-1.551	13.787	21.306	1.00	46.35
330	C	LEU	A	516	0.524	17.278	17.293	1.00	51.13

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TABLE 8

FGFR1 COORDINATE DATA FOR RESIDUES 506-578

331	CA	LEU	A	516	0.335	16.33	16.12	1.00	47.73
332	CB	LEU	A	516	-0.497	17.032	15.048	1.00	44.7
333	CD1	LEU	A	516	-1.758	17.046	12.927	1.00	39.43
334	CD2	LEU	A	516	0.559	16.084	12.984	1.00	42.51
335	CG	LEU	A	516	-0.752	16.277	13.747	1.00	42.26
336	N	LEU	A	516	-0.343	15.122	16.557	1.00	47.02
337	O	LEU	A	516	-0.183	17.194	18.302	1.00	50.3
338	C	LYS	A	517	0.8	20.324	17.958	1.00	60.52
339	CA	LYS	A	517	1.773	19.171	18.178	1.00	59.77
340	CB	LYS	A	517	3.214	19.675	18.062	1.00	62.36
341	CD	LYS	A	517	5.636	19.082	17.911	1.00	68.33
342	CE	LYS	A	517	6.729	18.1	18.309	1.00	72.52
343	CG	LYS	A	517	4.275	18.646	18.424	1.00	65.42
344	N	LYS	A	517	1.498	18.169	17.157	1.00	55.92
345	NZ	LYS	A	517	8.033	18.422	17.647	1.00	73.97
346	O	LYS	A	517	0.162	20.413	16.909	1.00	60.4
347	C	SER	A	518	0.078	23.226	17.61	1.00	64.5
348	CA	SER	A	518	-0.189	22.361	18.838	1.00	63.9
349	CB	SER	A	518	-0.108	23.216	20.106	1.00	64.23
350	N	SER	A	518	0.717	21.222	18.932	1.00	62.33
351	O	SER	A	518	-0.856	23.693	16.958	1.00	66.28
352	C	ASP	A	519	1.873	23.458	14.824	1.00	63.77
353	CA	ASP	A	519	1.733	24.231	16.135	1.00	64.64
354	CB	ASP	A	519	3.038	24.97	16.433	1.00	66.11
355	N	ASP	A	519	1.352	23.408	17.279	1.00	64.39
356	O	ASP	A	519	2.504	23.946	13.886	1.00	64.39
357	C	ALA	A	520	0.651	22.082	12.389	1.00	58.06
358	CA	ALA	A	520	1.369	21.434	13.56	1.00	60.2
359	CB	ALA	A	520	0.776	20.06	13.828	1.00	60.89
360	N	ALA	A	520	1.29	22.264	14.759	1.00	62.36
361	O	ALA	A	520	-0.428	22.648	12.545	1.00	58.32
362	C	THR	A	521	-0.184	21.512	9.287	1.00	54.3
363	CA	THR	A	521	0.67	22.552	10.005	1.00	54.91
364	CB	THR	A	521	1.772	22.989	9.053	1.00	53.6
365	CG2	THR	A	521	2.669	24.014	9.72	1.00	55.1
366	N	THR	A	521	1.249	21.983	11.211	1.00	55.83
367	O	THR	A	521	-0.184	20.338	9.651	1.00	54.57
368	OG1	THR	A	521	2.552	21.844	8.685	1.00	55.12
369	C	GLU	A	522	-0.798	19.992	6.81	1.00	52.04
370	CA	GLU	A	522	-1.708	21.043	7.452	1.00	52.87

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TABLE 8  
FGFR1 COORDINATE DATA FOR RESIDUES 506-578

371	CB	GLU	A	522	-2.476	21.81	6.372	1.00	53.64
372	N	GLU	A	522	-0.884	21.946	8.245	1.00	53.37
373	O	GLU	A	522	-1.212	18.858	6.587	1.00	53.06
374	C	LYS	A	523	1.692	18.396	6.976	1.00	44.09
375	CA	LYS	A	523	1.405	19.463	5.933	1.00	46.67
376	CB	LYS	A	523	2.694	20.212	5.572	1.00	48.82
377	CD	LYS	A	523	3.49	18.395	3.984	1.00	51.61
378	CE	LYS	A	523	4.709	17.645	3.463	1.00	54.47
379	CG	LYS	A	523	3.864	19.323	5.137	1.00	50.65
380	N	LYS	A	523	0.441	20.376	6.519	1.00	48.95
381	NZ	LYS	A	523	4.328	16.625	2.44	1.00	57.62
382	O	LYS	A	523	1.774	17.21	6.662	1.00	43.83
383	C	ASP	A	524	0.946	16.927	9.453	1.00	39.42
384	CA	ASP	A	524	2.102	17.916	9.32	1.00	41.96
385	CB	ASP	A	524	2.307	18.697	10.624	1.00	44.73
386	CG	ASP	A	524	3.625	19.468	10.651	1.00	49.12
387	N	ASP	A	524	1.836	18.831	8.221	1.00	42.69
388	O	ASP	A	524	1.155	15.739	9.734	1.00	38.37
389	OD1	ASP	A	524	4.579	19.074	9.94	1.00	50.64
390	OD2	ASP	A	524	3.714	20.463	11.404	1.00	52.03
391	C	LEU	A	525	-1.417	15.55	8.213	1.00	34.17
392	CA	LEU	A	525	-1.473	16.603	9.312	1.00	35.83
393	CB	LEU	A	525	-2.729	17.468	9.153	1.00	34.37
394	CD1	LEU	A	525	-4.186	15.733	10.294	1.00	35.99
395	CD2	LEU	A	525	-5.168	17.799	9.339	1.00	32.72
396	CG	LEU	A	525	-4.091	16.763	9.174	1.00	33.51
397	N	LEU	A	525	-0.27	17.429	9.254	1.00	38.1
398	O	LEU	A	525	-1.577	14.367	8.484	1.00	32.98
399	C	SER	A	526	-0.027	14.009	6.015	1.00	35.02
400	CA	SER	A	526	-1.059	15.107	5.82	1.00	36.14
401	CB	SER	A	526	-0.691	15.909	4.571	1.00	37.86
402	N	SER	A	526	-1.161	15.99	6.982	1.00	35.62
403	O	SER	A	526	-0.26	12.862	5.645	1.00	35.85
404	OG	SER	A	526	-1.736	16.798	4.232	1.00	48.77
405	C	ASP	A	527	1.744	12.3	7.808	1.00	31.04
406	CA	ASP	A	527	2.168	13.37	6.81	1.00	34.31
407	CB	ASP	A	527	3.471	14.046	7.236	1.00	34.5
408	CG	ASP	A	527	4.122	14.841	6.102	1.00	35.88
409	N	ASP	A	527	1.122	14.36	6.582	1.00	35.2
410	O	ASP	A	527	2.01	11.119	7.609	1.00	29.94

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TABLE 8

FGFR1 COORDINATE DATA FOR RESIDUES 506-578

411	OD1	ASP	A	527	3.765	14.645	4.919	1.00	36.2
412	OD2	ASP	A	527	5.001	15.674	6.404	1.00	42.28
413	C	LEU	A	528	-0.473	10.807	9.248	1.00	32.38
414	CA	LEU	A	528	0.578	11.749	9.868	1.00	32.76
415	CB	LEU	A	528	-0.006	12.488	11.089	1.00	30.45
416	CD1	LEU	A	528	0.673	10.692	12.715	1.00	31.93
417	CD2	LEU	A	528	-0.872	12.54	13.438	1.00	30.44
418	CG	LEU	A	528	-0.449	11.641	12.287	1.00	31.67
419	N	LEU	A	528	1.051	12.705	8.864	1.00	30.77
420	O	LEU	A	528	-0.505	9.61	9.554	1.00	31.87
421	C	ILE	A	529	-1.693	9.61	6.76	1.00	31.63
422	CA	ILE	A	529	-2.368	10.594	7.701	1.00	30.68
423	CB	ILE	A	529	-3.335	11.506	6.886	1.00	29.47
424	CD1	ILE	A	529	-5.144	13.315	7.137	1.00	32.37
425	CG1	ILE	A	529	-4.196	12.348	7.839	1.00	30.83
426	CG2	ILE	A	529	-4.233	10.666	5.983	1.00	29.84
427	N	ILE	A	529	-1.327	11.363	8.385	1.00	33.66
428	O	ILE	A	529	-2.007	8.424	6.772	1.00	31.35
429	C	SER	A	530	0.585	8.045	5.755	1.00	29.12
430	CA	SER	A	530	-0.024	9.24	5.027	1.00	32.48
431	CB	SER	A	530	1.085	10.032	4.326	1.00	37.28
432	N	SER	A	530	-0.754	10.101	5.956	1.00	33.17
433	O	SER	A	530	0.422	6.913	5.323	1.00	28.63
434	OG	SER	A	530	0.56	11.2	3.718	1.00	49.2
435	C	GLU	A	531	0.867	6.152	8.071	1.00	27.74
436	CA	GLU	A	531	1.874	7.209	7.629	1.00	27.55
437	CB	GLU	A	531	2.655	7.734	8.834	1.00	29.16
438	CD	GLU	A	531	4.045	7.064	10.89	1.00	30.35
439	CG	GLU	A	531	3.279	6.605	9.661	1.00	27.61
440	N	GLU	A	531	1.251	8.295	6.881	1.00	28.32
441	O	GLU	A	531	1.152	4.95	8.014	1.00	28.25
442	OE1	GLU	A	531	3.886	8.215	11.343	1.00	32.3
443	OE2	GLU	A	531	4.806	6.234	11.419	1.00	35.04
444	C	MET	A	532	-1.928	4.932	7.791	1.00	28.86
445	CA	MET	A	532	-1.367	5.72	8.991	1.00	28.98
446	CB	MET	A	532	-2.489	6.543	9.648	1.00	28.81
447	CE	MET	A	532	-5.44	7.876	9.48	1.00	27.27
448	CG	MET	A	532	-3.756	5.735	9.976	1.00	29.71
449	N	MET	A	532	-0.285	6.608	8.559	1.00	29.74
450	O	MET	A	532	-2.161	3.723	7.88	1.00	27.14

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451	SD	MET	A	532	-5.076	6.684	10.752	1.00	29.97
452	C	GLU	A	533	-1.693	3.957	4.956	1.00	28.24
453	CA	GLU	A	533	-2.674	5	5.464	1.00	28.27
454	CB	GLU	A	533	-2.943	6.052	4.394	1.00	25.76
455	CD	GLU	A	533	-5.407	6.208	5.034	1.00	27.98
456	CG	GLU	A	533	-4.112	6.971	4.746	1.00	29.45
457	N	GLU	A	533	-2.152	5.628	6.677	1.00	29.18
458	O	GLU	A	533	-2.083	2.863	4.553	1.00	27.95
459	OE1	GLU	A	533	-5.788	5.334	4.225	1.00	28.4
460	OE2	GLU	A	533	-6.053	6.489	6.067	1.00	32.98
461	C	MET	A	534	0.643	2.159	5.499	1.00	26.89
462	CA	MET	A	534	0.653	3.406	4.612	1.00	29.77
463	CB	MET	A	534	1.983	4.145	4.721	1.00	33.98
464	CE	MET	A	534	5.085	4.371	3.202	1.00	44.79
465	CG	MET	A	534	3.186	3.255	4.687	1.00	43.95
466	N	MET	A	534	-0.412	4.297	5.027	1.00	29.16
467	O	MET	A	534	0.785	1.036	5.016	1.00	27.11
468	SD	MET	A	534	3.884	3.145	3.079	1.00	50.26
469	C	MET	A	535	-0.747	0.326	7.398	1.00	26.29
470	CA	MET	A	535	0.434	1.246	7.733	1.00	25.7
471	CB	MET	A	535	0.324	1.745	9.176	1.00	28.01
472	CE	MET	A	535	1.328	4.26	11.715	1.00	29.02
473	CG	MET	A	535	1.606	2.37	9.734	1.00	27.91
474	N	MET	A	535	0.496	2.36	6.801	1.00	25.67
475	O	MET	A	535	-0.621	-0.904	7.487	1.00	25.46
476	SD	MET	A	535	1.575	2.547	11.562	1.00	29.83
477	C	LYS	A	536	-2.801	-0.71	5.426	1.00	24.85
478	CA	LYS	A	536	-3.091	0.147	6.656	1.00	27.33
479	CB	LYS	A	536	-4.268	1.07	6.326	1.00	25.11
480	CD	LYS	A	536	-5.886	2.815	7.029	1.00	21.87
481	CE	LYS	A	536	-6.475	3.584	8.182	1.00	21.93
482	CG	LYS	A	536	-4.909	1.761	7.508	1.00	23.65
483	N	LYS	A	536	-1.893	0.918	7.036	1.00	27.3
484	NZ	LYS	A	536	-7.462	4.567	7.701	1.00	23.58
485	O	LYS	A	536	-3.11	-1.896	5.393	1.00	27.16
486	C	MET	A	537	-0.885	-1.956	3.446	1.00	26.98
487	CA	MET	A	537	-1.875	-0.824	3.193	1.00	28.12
488	CB	MET	A	537	-1.305	0.135	2.14	1.00	29.73
489	CE	MET	A	537	-2.96	-0.029	-0.814	1.00	35.96
490	CG	MET	A	537	-2.29	1.162	1.592	1.00	35.71

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491	N	MET	A	537	-2.206	-0.103	4.413	1.00	27.18
492	O	MET	A	537	-1.088	-3.066	2.969	1.00	25.89
493	SD	MET	A	537	-3.729	0.463	0.72	1.00	42.08
494	C	ILE	A	538	0.753	-3.924	5.268	1.00	25.7
495	CA	ILE	A	538	1.217	-2.668	4.52	1.00	25.59
496	CB	ILE	A	538	2.438	-1.995	5.252	1.00	25.01
497	CD1	ILE	A	538	4.37	-0.384	4.898	1.00	27.43
498	CG1	ILE	A	538	3.206	-1.114	4.271	1.00	24.2
499	CG2	ILE	A	538	3.41	-3.034	5.83	1.00	24.96
500	N	ILE	A	538	0.169	-1.675	4.215	1.00	27.37
501	O	ILE	A	538	1.268	-5.023	5.033	1.00	26.08
502	C	GLY	A	539	0.186	-5.273	8.139	1.00	26.51
503	CA	GLY	A	539	-0.658	-4.955	6.911	1.00	24.86
504	N	GLY	A	539	-0.199	-3.778	6.184	1.00	26.04
505	O	GLY	A	539	1.211	-4.633	8.388	1.00	24.95
506	C	LYS	A	540	1.606	-7.675	10.012	1.00	24.49
507	CA	LYS	A	540	0.469	-6.689	10.09	1.00	26.22
508	CB	LYS	A	540	-0.544	-7.261	11.083	1.00	27.34
509	CD	LYS	A	540	-2.522	-6.981	12.55	1.00	40.39
510	CE	LYS	A	540	-3.569	-5.995	13.091	1.00	43.85
511	CG	LYS	A	540	-1.573	-6.298	11.576	1.00	33.86
512	N	LYS	A	540	-0.196	-6.323	8.854	1.00	25.35
513	NZ	LYS	A	540	-2.972	-4.89	13.906	1.00	43.95
514	O	LYS	A	540	1.629	-8.576	9.185	1.00	26.41
515	C	HIS	A	541	4.222	-8.313	12.482	1.00	26.13
516	CA	HIS	A	541	3.664	-8.404	11.082	1.00	25.69
517	CB	HIS	A	541	4.777	-8.177	10.054	1.00	22.01
518	CD2	HIS	A	541	5.795	-10.483	9.478	1.00	22.4
519	CE1	HIS	A	541	7.61	-10.347	10.702	1.00	24.83
520	CG	HIS	A	541	5.796	-9.269	10.07	1.00	23.48
521	N	HIS	A	541	2.546	-7.504	10.928	1.00	24.97
522	ND1	HIS	A	541	6.955	-9.207	10.822	1.00	21.83
523	NE2	HIS	A	541	6.934	-11.137	9.894	1.00	27.22
524	O	HIS	A	541	4.363	-7.22	13.044	1.00	27.29
525	C	LYS	A	542	6.34	-8.682	14.618	1.00	27.93
526	CA	LYS	A	542	5.119	-9.574	14.375	1.00	30.26
527	CB	LYS	A	542	5.455	-11.034	14.641	1.00	31.63
528	CD	LYS	A	542	6.345	-12.763	16.155	1.00	49.91
529	CE	LYS	A	542	7.067	-13.339	14.918	1.00	56.28
530	CG	LYS	A	542	6.073	-11.292	15.995	1.00	42.08

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531	N	LYS	A	542	4.556	-9.458	13.048	1.00	26.79
532	NZ	LYS	A	542	7.57	-14.735	15.13	1.00	60.35
533	O	LYS	A	542	6.491	-8.135	15.692	1.00	27.54
534	C	ASN	A	543	8.365	-6.226	13.231	1.00	25.23
535	CA	ASN	A	543	8.347	-7.659	13.736	1.00	25.53
536	CB	ASN	A	543	9.565	-8.446	13.244	1.00	25.81
537	CG	ASN	A	543	9.7	-9.78	13.951	1.00	22.78
538	N	ASN	A	543	7.136	-8.467	13.575	1.00	27.38
539	ND2	ASN	A	543	9.966	-9.746	15.247	1.00	25.54
540	O	ASN	A	543	9.411	-5.71	12.847	1.00	24.94
541	OD1	ASN	A	543	9.511	-10.829	13.343	1.00	28.02
542	C	ILE	A	544	6.075	-3.59	13.889	1.00	22.45
543	CA	ILE	A	544	7.07	-4.178	12.879	1.00	22.3
544	CB	ILE	A	544	6.529	-3.978	11.412	1.00	25.58
545	CD1	ILE	A	544	4.442	-4.123	9.915	1.00	22.9
546	CG1	ILE	A	544	5.055	-4.423	11.287	1.00	26.22
547	CG2	ILE	A	544	7.399	-4.743	10.409	1.00	24.01
548	N	ILE	A	544	7.206	-5.578	13.263	1.00	24.4
549	O	ILE	A	544	5.354	-4.333	14.563	1.00	21.36
550	C	ILE	A	545	3.877	-1.604	14.176	1.00	26.11
551	CA	ILE	A	545	5.161	-1.646	14.992	1.00	25.87
552	CB	ILE	A	545	5.595	-0.203	15.369	1.00	26.84
553	CD1	ILE	A	545	6.584	-0.787	17.67	1.00	23.96
554	CG1	ILE	A	545	6.841	-0.237	16.271	1.00	25.55
555	CG2	ILE	A	545	4.45	0.551	16.049	1.00	21.59
556	N	ILE	A	545	6.107	-2.282	14.079	1.00	23.71
557	O	ILE	A	545	3.834	-0.992	13.112	1.00	25.86
558	C	ASN	A	546	0.571	-1.275	14.356	1.00	26.78
559	CA	ASN	A	546	1.574	-2.343	13.953	1.00	25.33
560	CB	ASN	A	546	0.925	-3.72	14.142	1.00	25.52
561	CG	ASN	A	546	1.723	-4.827	13.519	1.00	21.5
562	N	ASN	A	546	2.845	-2.279	14.663	1.00	24.88
563	ND2	ASN	A	546	2.281	-5.685	14.342	1.00	21.52
564	O	ASN	A	546	0.612	-0.737	15.468	1.00	28.75
565	OD1	ASN	A	546	1.826	-4.919	12.307	1.00	23.96
566	C	LEU	A	547	-2.416	-0.773	14.387	1.00	27.12
567	CA	LEU	A	547	-1.358	0.024	13.619	1.00	27.39
568	CB	LEU	A	547	-1.938	0.477	12.278	1.00	24.89
569	CD1	LEU	A	547	-2.758	2.76	12.925	1.00	24.31
570	CD2	LEU	A	547	-3.773	1.551	10.942	1.00	24.2

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571	CG	LEU	A	547	-3.161	1.395	12.35	1.00	23.83
572	N	LEU	A	547	-0.292	-0.942	13.407	1.00	27.36
573	O	LEU	A	547	-2.648	-1.96	14.092	1.00	25.71
574	C	LEU	A	548	-5.373	-0.116	16.042	1.00	26.77
575	CA	LEU	A	548	-4.022	-0.778	16.219	1.00	27.08
576	CB	LEU	A	548	-3.628	-0.733	17.703	1.00	24.94
577	CD1	LEU	A	548	-2.192	-1.414	19.597	1.00	25.58
578	CD2	LEU	A	548	-2.365	-2.906	17.628	1.00	23.71
579	CG	LEU	A	548	-2.337	-1.463	18.096	1.00	25.5
580	N	LEU	A	548	-3.005	-0.142	15.395	1.00	27.97
581	O	LEU	A	548	-6.397	-0.742	16.264	1.00	27.49
582	C	GLY	A	549	-6.423	3.33	15.368	1.00	26.68
583	CA	GLY	A	549	-6.645	1.848	15.519	1.00	25.65
584	N	GLY	A	549	-5.381	1.158	15.681	1.00	25.23
585	O	GLY	A	549	-5.271	3.777	15.286	1.00	28.71
586	C	ALA	A	550	-8.644	6.274	15.691	1.00	25.72
587	CA	ALA	A	550	-7.409	5.544	15.202	1.00	24.63
588	CB	ALA	A	550	-7.17	5.905	13.726	1.00	21.88
589	N	ALA	A	550	-7.508	4.098	15.354	1.00	25.64
590	O	ALA	A	550	-9.748	5.72	15.69	1.00	24.43
591	C	CYS	A	551	-9.341	9.586	15.524	1.00	28.52
592	CA	CYS	A	551	-9.492	8.432	16.527	1.00	26.99
593	CB	CYS	A	551	-9.257	8.924	17.962	1.00	26.22
594	N	CYS	A	551	-8.433	7.525	16.097	1.00	25
595	O	CYS	A	551	-8.366	10.348	15.575	1.00	28.59
596	SG	CYS	A	551	-9.338	7.651	19.241	1.00	32.33
597	C	THR	A	552	-11.325	11.658	13.507	1.00	33.36
598	CA	THR	A	552	-10.17	10.671	13.513	1.00	31.38
599	CB	THR	A	552	-10.119	9.995	12.106	1.00	30.1
600	CG2	THR	A	552	-9.008	8.967	12.063	1.00	28.72
601	N	THR	A	552	-10.246	9.654	14.555	1.00	28.57
602	O	THR	A	552	-11.271	12.698	12.847	1.00	32.35
603	OG1	THR	A	552	-11.365	9.329	11.823	1.00	29.38
604	C	GLN	A	553	-13.659	13.076	15.432	1.00	40.85
605	CA	GLN	A	553	-13.569	12.158	14.231	1.00	38.9
606	CB	GLN	A	553	-14.824	11.287	14.131	1.00	36.78
607	CD	GLN	A	553	-14.746	11.23	11.585	1.00	38.71
608	CG	GLN	A	553	-14.886	10.417	12.864	1.00	37.42
609	N	GLN	A	553	-12.386	11.316	14.22	1.00	35.68
610	NE2	GLN	A	553	-13.755	10.887	10.767	1.00	38.17



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611	O	GLN	A	553	-13.169	12.746	16.502	1.00	41.24
612	OE1	GLN	A	553	-15.523	12.154	11.334	1.00	38.58
613	C	ASP	A	554	-13.356	15.375	17.291	1.00	48.16
614	CA	ASP	A	554	-14.468	15.256	16.247	1.00	47.91
615	CB	ASP	A	554	-15.803	14.99	16.946	1.00	50.37
616	CG	ASP	A	554	-16.99	15.207	16.033	1.00	55.94
617	N	ASP	A	554	-14.249	14.25	15.212	1.00	44.66
618	O	ASP	A	554	-13.564	15.083	18.479	1.00	49.45
619	OD1	ASP	A	554	-16.975	14.709	14.889	1.00	57.62
620	OD2	ASP	A	554	-17.946	15.884	16.466	1.00	63.43
621	C	GLY	A	555	-9.734	15.714	17.06	1.00	40.8
622	CA	GLY	A	555	-11.063	15.952	17.747	1.00	42.42
623	N	GLY	A	555	-12.181	15.798	16.841	1.00	44.94
624	O	GLY	A	555	-9.695	15.455	15.859	1.00	40.53
625	C	PRO	A	556	-7.102	14.195	16.76	1.00	37.06
626	CA	PRO	A	556	-7.268	15.604	17.291	1.00	38.65
627	CB	PRO	A	556	-6.402	15.786	18.533	1.00	39.19
628	CD	PRO	A	556	-8.598	16.069	19.247	1.00	40.79
629	CG	PRO	A	556	-7.228	16.634	19.421	1.00	42.75
630	N	PRO	A	556	-8.624	15.804	17.796	1.00	39.91
631	O	PRO	A	556	-7.564	13.241	17.38	1.00	37.33
632	C	LEU	A	557	-5.271	11.959	15.958	1.00	33.73
633	CA	LEU	A	557	-6.173	12.771	15.033	1.00	34.61
634	CB	LEU	A	557	-5.497	12.939	13.661	1.00	31.67
635	CD1	LEU	A	557	-6.108	10.682	12.692	1.00	25.86
636	CD2	LEU	A	557	-4.254	12.039	11.689	1.00	24.56
637	CG	LEU	A	557	-4.974	11.667	12.967	1.00	30.04
638	N	LEU	A	557	-6.414	14.07	15.635	1.00	36.64
639	O	LEU	A	557	-4.228	12.446	16.402	1.00	34.58
640	C	TYR	A	558	-4.622	8.619	16.344	1.00	31.1
641	CA	TYR	A	558	-4.91	9.88	17.14	1.00	31.85
642	CB	TYR	A	558	-5.631	9.53	18.454	1.00	33.06
643	CD1	TYR	A	558	-4.876	11.776	19.346	1.00	38.15
644	CD2	TYR	A	558	-6.647	10.638	20.496	1.00	35.4
645	CE1	TYR	A	558	-4.961	12.835	20.239	1.00	40.71
646	CE2	TYR	A	558	-6.743	11.697	21.4	1.00	38.4
647	CG	TYR	A	558	-5.715	10.665	19.454	1.00	34.91
648	CZ	TYR	A	558	-5.897	12.795	21.262	1.00	41.95
649	N	TYR	A	558	-5.709	10.757	16.308	1.00	32.12
650	O	TYR	A	558	-5.543	7.954	15.855	1.00	31.27

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651	OH	TYR	A	558	-5.988	13.874	22.122	1.00	43.69
652	C	VAL	A	559	-2.41	6.23	16.505	1.00	25.24
653	CA	VAL	A	559	-2.935	7.146	15.418	1.00	26.75
654	CB	VAL	A	559	-1.838	7.427	14.368	1.00	28.9
655	CG1	VAL	A	559	-1.488	6.14	13.63	1.00	26.37
656	CG2	VAL	A	559	-2.312	8.495	13.377	1.00	28.88
657	N	VAL	A	559	-3.343	8.346	16.131	1.00	28.71
658	O	VAL	A	559	-1.383	6.507	17.118	1.00	27.85
659	C	ILE	A	560	-2.009	3.056	17.279	1.00	26.35
660	CA	ILE	A	560	-2.843	4.21	17.828	1.00	25.21
661	CB	ILE	A	560	-4.14	3.67	18.481	1.00	24.4
662	CD1	ILE	A	560	-6.477	4.518	19.003	1.00	25.58
663	CG1	ILE	A	560	-5.03	4.856	18.88	1.00	22.47
664	CG2	ILE	A	560	-3.802	2.82	19.716	1.00	21.06
665	N	ILE	A	560	-3.169	5.178	16.785	1.00	25.77
666	O	ILE	A	560	-2.441	2.315	16.381	1.00	26.85
667	C	VAL	A	561	0.606	1.026	18.552	1.00	25.89
668	CA	VAL	A	561	0.091	1.845	17.364	1.00	27.03
669	CB	VAL	A	561	1.279	2.43	16.529	1.00	24.28
670	CG1	VAL	A	561	0.751	3.196	15.334	1.00	18.51
671	CG2	VAL	A	561	2.14	3.345	17.387	1.00	25.72
672	N	VAL	A	561	-0.804	2.902	17.816	1.00	27.59
673	O	VAL	A	561	0.368	1.373	19.717	1.00	25.9
674	C	GLU	A	562	2.843	-0.279	20.169	1.00	27.29
675	CA	GLU	A	562	1.807	-0.95	19.28	1.00	25.07
676	CB	GLU	A	562	2.368	-2.225	18.67	1.00	23.84
677	CD	GLU	A	562	1.833	-4.397	17.513	1.00	27.74
678	CG	GLU	A	562	1.286	-3.179	18.226	1.00	25.17
679	N	GLU	A	562	1.28	-0.077	18.249	1.00	24.52
680	O	GLU	A	562	3.609	0.563	19.726	1.00	26.25
681	OE1	GLU	A	562	2.848	-4.266	16.803	1.00	31.28
682	OE2	GLU	A	562	1.24	-5.488	17.641	1.00	30.23
683	C	TYR	A	563	4.879	-1.069	22.718	1.00	31.38
684	CA	TYR	A	563	3.713	-0.131	22.452	1.00	32.7
685	CB	TYR	A	563	2.932	0.123	23.745	1.00	33.73
686	CD1	TYR	A	563	4.597	1.671	24.853	1.00	34.42
687	CD2	TYR	A	563	3.772	-0.196	26.098	1.00	33.18
688	CE1	TYR	A	563	5.367	2.066	25.946	1.00	37.31
689	CE2	TYR	A	563	4.533	0.185	27.189	1.00	34.92
690	CG	TYR	A	563	3.79	0.536	24.917	1.00	35.05

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FGFR1 COORDINATE DATA FOR RESIDUES 506-578

691	CZ	TYR	A	563	5.322	1.314	27.108	1.00	36.85
692	N	TYR	A	563	2.818	-0.855	21.442	1.00	30.89
693	O	TYR	A	563	4.702	-2.279	22.886	1.00	30.71
694	OH	TYR	A	563	6.072	1.679	28.196	1.00	44.45
695	C	ALA	A	564	7.853	-0.653	24.327	1.00	32
696	CA	ALA	A	564	7.311	-1.225	23.022	1.00	32.85
697	CB	ALA	A	564	8.303	-0.981	21.862	1.00	30.78
698	N	ALA	A	564	6.072	-0.489	22.765	1.00	32.48
699	O	ALA	A	564	8.481	0.41	24.322	1.00	33.34
700	C	SER	A	565	9.536	-0.788	27.042	1.00	35.31
701	CA	SER	A	565	8.033	-0.871	26.763	1.00	35.13
702	CB	SER	A	565	7.382	-1.709	27.861	1.00	30.99
703	N	SER	A	565	7.618	-1.353	25.436	1.00	33.67
704	O	SER	A	565	9.96	0.009	27.889	1.00	37.53
705	OG	SER	A	565	7.671	-3.073	27.629	1.00	37.59
706	C	LYS	A	566	12.593	-0.616	25.682	1.00	35.75
707	CA	LYS	A	566	11.784	-1.557	26.563	1.00	34.2
708	CB	LYS	A	566	12.329	-2.987	26.525	1.00	32.88
709	CD	LYS	A	566	12.157	-5.288	27.529	1.00	36.32
710	CE	LYS	A	566	11.723	-6.026	28.783	1.00	37.39
711	CG	LYS	A	566	11.661	-3.868	27.567	1.00	30.58
712	N	LYS	A	566	10.342	-1.569	26.325	1.00	34.95
713	NZ	LYS	A	566	12.227	-7.429	28.794	1.00	40.69
714	O	LYS	A	566	13.81	-0.751	25.58	1.00	38.56
715	C	GLY	A	567	13.238	0.878	22.944	1.00	32.5
716	CA	GLY	A	567	12.588	1.335	24.239	1.00	34.94
717	N	GLY	A	567	11.91	0.343	25.059	1.00	36.93
718	O	GLY	A	567	12.954	-0.204	22.448	1.00	32.15
719	C	ASN	A	568	15.907	0.396	21.336	1.00	33.66
720	CA	ASN	A	568	14.76	1.37	21.129	1.00	34.14
721	CB	ASN	A	568	15.187	2.618	20.34	1.00	33.99
722	CG	ASN	A	568	16.398	3.318	20.92	1.00	34.79
723	N	ASN	A	568	14.093	1.721	22.372	1.00	33.48
724	ND2	ASN	A	568	16.299	4.624	21.046	1.00	38.03
725	O	ASN	A	568	16.461	0.307	22.428	1.00	34.84
726	OD1	ASN	A	568	17.426	2.708	21.188	1.00	34.27
727	C	LEU	A	569	18.706	-0.798	20.762	1.00	30.93
728	CA	LEU	A	569	17.332	-1.311	20.304	1.00	31.46
729	CB	LEU	A	569	17.437	-2.007	18.935	1.00	30.72
730	CD1	LEU	A	569	18.275	-4.23	19.822	1.00	29.97

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FGFR1 COORDINATE DATA FOR RESIDUES 506-578

731	CD2	LEU	A	569	18.299	-3.724	17.34	1.00	27.44
732	CG	LEU	A	569	18.45	-3.143	18.748	1.00	30.5
733	N	LEU	A	569	16.273	-0.31	20.269	1.00	31.86
734	O	LEU	A	569	19.406	-1.497	21.488	1.00	28.28
735	C	ARG	A	570	20.44	1.034	22.282	1.00	35.38
736	CA	ARG	A	570	20.387	0.962	20.746	1.00	33.95
737	CB	ARG	A	570	20.603	2.359	20.146	1.00	32.96
738	CD	ARG	A	570	21.961	4.507	20.37	1.00	39.64
739	CG	ARG	A	570	21.879	3.025	20.665	1.00	37.53
740	CZ	ARG	A	570	20.377	5.599	21.952	1.00	52.42
741	N	ARG	A	570	19.093	0.404	20.341	1.00	31.35
742	NE	ARG	A	570	20.738	5.227	20.721	1.00	50.64
743	NH1	ARG	A	570	21.136	5.331	23.017	1.00	50.35
744	NH2	ARG	A	570	19.237	6.26	22.113	1.00	54.27
745	O	ARG	A	570	21.351	0.49	22.919	1.00	35.47
746	C	GLU	A	571	19.315	0.456	25.007	1.00	34.99
747	CA	GLU	A	571	19.315	1.815	24.31	1.00	36.22
748	CB	GLU	A	571	18.027	2.564	24.646	1.00	38.71
749	CD	GLU	A	571	16.638	4.649	24.295	1.00	50.18
750	CG	GLU	A	571	18.012	4.007	24.189	1.00	45.81
751	N	GLU	A	571	19.43	1.672	22.864	1.00	35.25
752	O	GLU	A	571	20.028	0.244	25.997	1.00	35.42
753	OE1	GLU	A	571	15.633	3.907	24.416	1.00	54.14
754	OE2	GLU	A	571	16.56	5.898	24.24	1.00	51.58
755	C	TYR	A	572	19.703	-2.558	25.055	1.00	34.39
756	CA	TYR	A	572	18.37	-1.815	24.992	1.00	31.93
757	CB	TYR	A	572	17.388	-2.575	24.098	1.00	30.34
758	CD1	TYR	A	572	16.195	-4.435	25.312	1.00	30.25
759	CD2	TYR	A	572	17.939	-5.022	23.783	1.00	25.43
760	CE1	TYR	A	572	15.962	-5.77	25.573	1.00	30.72
761	CE2	TYR	A	572	17.713	-6.363	24.038	1.00	25.24
762	CG	TYR	A	572	17.183	-4.035	24.413	1.00	27.61
763	CZ	TYR	A	572	16.719	-6.728	24.941	1.00	29.85
764	N	TYR	A	572	18.514	-0.459	24.471	1.00	33.65
765	O	TYR	A	572	19.981	-3.294	26.014	1.00	34.52
766	OH	TYR	A	572	16.48	-8.052	25.229	1.00	33.15
767	C	LEU	A	573	22.798	-2.421	24.942	1.00	37.08
768	CA	LEU	A	573	21.811	-3.058	23.964	1.00	34.94
769	CB	LEU	A	573	22.372	-3.024	22.534	1.00	32.14
770	CD1	LEU	A	573	22.185	-3.502	20.083	1.00	26.59

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FGFR1 COORDINATE DATA FOR RESIDUES 506-578

771	CD2	LEU	A	573	21.927	-5.343	21.716	1.00	28.48
772	CG	LEU	A	573	21.685	-3.88	21.461	1.00	28.46
773	N	LEU	A	573	20.518	-2.388	24.02	1.00	33.7
774	O	LEU	A	573	23.501	-3.121	25.679	1.00	36.56
775	C	GLN	A	574	23.499	-0.706	27.318	1.00	41.46
776	CA	GLN	A	574	23.738	-0.377	25.846	1.00	40.26
777	CB	GLN	A	574	23.642	1.13	25.584	1.00	40.16
778	CD	GLN	A	574	24.027	3.001	23.893	1.00	44.45
779	CG	GLN	A	574	24.241	1.539	24.236	1.00	42.29
780	N	GLN	A	574	22.821	-1.093	24.971	1.00	37.9
781	NE2	GLN	A	574	24.61	3.432	22.789	1.00	46.58
782	O	GLN	A	574	24.447	-0.954	28.069	1.00	41.68
783	OE1	GLN	A	574	23.331	3.729	24.595	1.00	47.62
784	C	ALA	A	575	22.188	-2.527	29.508	1.00	40.86
785	CA	ALA	A	575	21.843	-1.103	29.071	1.00	39.38
786	CB	ALA	A	575	20.352	-0.834	29.263	1.00	35.91
787	N	ALA	A	575	22.228	-0.801	27.698	1.00	40.68
788	O	ALA	A	575	22.094	-2.85	30.696	1.00	43.7
789	C	ARG	A	576	24.41	-5.084	28.708	1.00	38.88
790	CA	ARG	A	576	22.038	-4.747	28.895	1.00	37.74
791	CB	ARG	A	576	22.031	-5.702	28.125	1.00	38.03
792	CD	ARG	A	576	19.611	-6.257	27.675	1.00	36.8
793	CG	ARG	A	576	20.59	-5.564	28.58	1.00	37.86
794	CZ	ARG	A	576	17.569	-5.133	28.5	1.00	36.46
795	N	ARG	A	576	22.597	-3.373	28.567	1.00	38.67
796	NE	ARG	A	576	18.257	-6.237	28.231	1.00	34.25
797	NH1	ARG	A	576	18.101	-3.938	28.279	1.00	35.55
798	NH2	ARG	A	576	16.313	-5.221	28.924	1.00	41.01
799	O	ARG	A	576	24.799	-6.259	28.712	1.00	40.03
800	C	ARG	A	577	27.231	-4.566	29.779	1.00	40.4
801	CA	ARG	A	577	26.668	-4.203	28.412	1.00	38.74
802	CB	ARG	A	577	27.306	-2.881	28.001	1.00	35.53
803	CD	ARG	A	577	27.699	-1.109	26.332	1.00	36.13
804	CG	ARG	A	577	26.968	-2.404	26.618	1.00	36.41
805	CZ	ARG	A	577	28.286	0.283	24.374	1.00	39.66
806	N	ARG	A	577	25.228	-4.045	28.562	1.00	38.88
807	NE	ARG	A	577	27.756	-0.818	24.902	1.00	38.29
808	NH1	ARG	A	577	28.814	1.219	25.156	1.00	39.78
809	NH2	ARG	A	577	28.294	0.447	23.056	1.00	38.4
810	O	ARG	A	577	26.669	-4.177	30.802	1.00	37.88

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TABLE 8

FGFR1 COORDINATE DATA FOR RESIDUES 506-578

811	C	PRO	A	578	29.488	-4.443	31.761	1.00	45.42
812	CA	PRO	A	578	28.917	-5.707	31.114	1.00	45.3
813	CB	PRO	A	578	30.014	-6.705	30.723	1.00	45.22
814	CD	PRO	A	578	29.046	-6.003	28.721	1.00	44.61
815	CG	PRO	A	578	30.396	-6.267	29.348	1.00	44.97
816	N	PRO	A	578	28.326	-5.342	29.822	1.00	42.78
817	O	PRO	A	578	29.82	-3.477	31.066	1.00	43.66

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TABLE 9  
FGFR1 COORDINATE DATA FOR RESIDUES 592-647

ATO M	ATOM TYPE	RESIDUE	PROTEIN #	#	X	Y	Z	OCC	B
825	C	GLU	A	592	21.442	-6.393	32.31	1.00	64.11
826	CA	GLU	A	592	20.621	-5.12	32.5	1.00	64.91
827	CB	GLU	A	592	21.014	-4.444	33.816	1.00	67.85
828	N	GLU	A	592	19.176	-5.368	32.459	1.00	64.55
829	O	GLU	A	592	22.636	-6.331	32.018	1.00	65.76
830	C	GLU	A	593	22.104	-8.929	30.924	1.00	59.46
831	CA	GLU	A	593	21.483	-8.83	32.317	1.00	61.45
832	CB	GLU	A	593	20.512	-9.988	32.539	1.00	61.42
833	N	GLU	A	593	20.799	-7.545	32.474	1.00	62.56
834	O	GLU	A	593	21.467	-8.599	29.923	1.00	60.27
835	C	GLN	A	594	23.306	-10.409	28.63	1.00	52.2
836	CA	GLN	A	594	24.079	-9.53	29.617	1.00	55.01
837	CB	GLN	A	594	25.477	-10.118	29.866	1.00	55.3
838	CD	GLN	A	594	27.666	-9.953	31.159	1.00	59.97
839	CG	GLN	A	594	26.423	-9.216	30.654	1.00	57.01
840	N	GLN	A	594	23.353	-9.381	30.875	1.00	58.03
841	NE2	GLN	A	594	28.102	-9.603	32.368	1.00	59.24
842	O	GLN	A	594	22.555	-11.31	29.02	1.00	51.5
843	OE1	GLN	A	594	28.22	-10.829	30.48	1.00	59.29
844	C	LEU	A	595	23.757	-11.89	25.83	1.00	43.33
845	CA	LEU	A	595	22.794	-10.832	26.288	1.00	44.99
846	CB	LEU	A	595	22.468	-9.897	25.125	1.00	41.52
847	CD1	LEU	A	595	21.625	-7.564	24.658	1.00	36.48
848	CD2	LEU	A	595	20.068	-9.381	25.496	1.00	35.36
849	CG	LEU	A	595	21.474	-8.806	25.526	1.00	39.57
850	N	LEU	A	595	23.448	-10.09	27.35	1.00	49.68
851	O	LEU	A	595	24.957	-11.648	25.769	1.00	43.48
852	C	SER	A	596	24.33	-13.926	23.59	1.00	41.76
853	CA	SER	A	596	24.09	-14.151	25.079	1.00	41.97
854	CB	SER	A	596	23.415	-15.505	25.305	1.00	40.99
855	N	SER	A	596	23.242	-13.081	25.557	1.00	43.04
856	O	SER	A	596	23.659	-13.101	22.96	1.00	41.96
857	OG	SER	A	596	22.198	-15.606	24.591	1.00	37.99
858	C	SER	A	597	24.315	-14.921	20.827	1.00	38.01
859	CA	SER	A	597	25.56	-14.525	21.613	1.00	39.75
860	CB	SER	A	597	26.734	-15.409	21.223	1.00	40.99
861	N	SER	A	597	25.289	-14.647	23.028	1.00	40.04
862	O	SER	A	597	24.035	-14.341	19.787	1.00	37.85
863	OG	SER	A	597	27.865	-15.078	22.002	1.00	49.55

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TABLE 9  
FGFR1 COORDINATE DATA FOR RESIDUES 592-647

864	C	LYS	A	598	21.331	-15.195	20.683	1.00	37.05
865	CA	LYS	A	598	22.364	-16.319	20.626	1.00	35.53
866	CB	LYS	A	598	21.786	-17.598	21.225	1.00	36.68
867	CD	LYS	A	598	20.163	-19.511	20.845	1.00	39.94
868	CE	LYS	A	598	19.81	-20.602	19.844	1.00	46.08
869	CG	LYS	A	598	20.991	-18.419	20.2	1.00	40.2
870	N	LYS	A	598	23.564	-15.902	21.321	1.00	35.72
871	NZ	LYS	A	598	21.007	-21.381	19.398	1.00	44.68
872	O	LYS	A	598	20.593	-14.972	19.712	1.00	37.54
873	C	ASP	A	599	20.621	-12.315	20.925	1.00	32.49
874	CA	ASP	A	599	20.369	-13.363	21.983	1.00	33.79
875	CB	ASP	A	599	20.55	-12.69	23.342	1.00	37.46
876	CG	ASP	A	599	19.944	-13.478	24.482	1.00	39.98
877	N	ASP	A	599	21.304	-14.472	21.804	1.00	34.94
878	O	ASP	A	599	19.684	-11.779	20.324	1.00	30.34
879	OD1	ASP	A	599	19.187	-14.442	24.233	1.00	42.34
880	OD2	ASP	A	599	20.22	-13.105	25.641	1.00	42.09
881	C	LEU	A	600	21.947	-11.398	18.318	1.00	30.63
882	CA	LEU	A	600	22.314	-11.007	19.755	1.00	31.96
883	CB	LEU	A	600	23.813	-10.744	19.896	1.00	32.06
884	CD1	LEU	A	600	25.786	-9.979	21.284	1.00	30.28
885	CD2	LEU	A	600	23.545	-8.87	21.508	1.00	28.48
886	CG	LEU	A	600	24.258	-10.184	21.256	1.00	31.04
887	N	LEU	A	600	21.898	-12.006	20.732	1.00	30.67
888	O	LEU	A	600	21.341	-10.613	17.582	1.00	29.38
889	C	VAL	A	601	20.457	-13.185	16.389	1.00	29.25
890	CA	VAL	A	601	21.971	-13.116	16.601	1.00	29.3
891	CB	VAL	A	601	22.612	-14.495	16.344	1.00	31.41
892	CG1	VAL	A	601	22.396	-14.919	14.906	1.00	31.14
893	CG2	VAL	A	601	24.104	-14.436	16.642	1.00	31.39
894	N	VAL	A	601	22.28	-12.628	17.936	1.00	30.02
895	O	VAL	A	601	19.974	-12.923	15.287	1.00	27.77
896	C	SER	A	602	17.676	-12.192	17.138	1.00	28.93
897	CA	SER	A	602	18.252	-13.587	17.374	1.00	29.33
898	CB	SER	A	602	17.673	-14.17	18.656	1.00	31.2
899	N	SER	A	602	19.712	-13.512	17.446	1.00	29.47
900	O	SER	A	602	16.669	-12.037	16.44	1.00	26.88
901	OG	SER	A	602	16.257	-14.044	18.665	1.00	35.84
902	C	CYS	A	603	18.001	-9.409	16.12	1.00	28.48
903	CA	CYS	A	603	17.896	-9.796	17.6	1.00	28.5



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FGFR1 COORDINATE DATA FOR RESIDUES 592-647

904	CB	CYS	A	603	18.82	-8.888	18.423	1.00	28.15
905	N	CYS	A	603	18.294	-11.191	17.76	1.00	28.65
906	O	CYS	A	603	17.092	-8.791	15.561	1.00	26.73
907	SG	CYS	A	603	18.603	-7.132	18.164	0.50	22.53
908	C	ALA	A	604	18.339	-10.215	13.226	1.00	25.71
909	CA	ALA	A	604	19.364	-9.495	14.084	1.00	26.36
910	CB	ALA	A	604	20.762	-9.942	13.692	1.00	23.76
911	N	ALA	A	604	19.118	-9.78	15.497	1.00	27.36
912	O	ALA	A	604	17.796	-9.647	12.28	1.00	26.27
913	C	TYR	A	605	15.738	-11.632	12.747	1.00	26.08
914	CA	TYR	A	605	17.133	-12.272	12.793	1.00	27.81
915	CB	TYR	A	605	17.053	-13.672	13.398	1.00	27.14
916	CD1	TYR	A	605	16.047	-15.159	11.612	1.00	31.24
917	CD2	TYR	A	605	14.759	-14.716	13.583	1.00	31.22
918	CE1	TYR	A	605	15.023	-15.976	11.123	1.00	30.91
919	CE2	TYR	A	605	13.737	-15.528	13.106	1.00	31.94
920	CG	TYR	A	605	15.93	-14.522	12.849	1.00	30.78
921	CZ	TYR	A	605	13.877	-16.153	11.877	1.00	31.52
922	N	TYR	A	605	18.102	-11.481	13.535	1.00	25.48
923	O	TYR	A	605	15.135	-11.539	11.679	1.00	26.76
924	OH	TYR	A	605	12.871	-16.961	11.421	1.00	32.71
925	C	GLN	A	606	13.829	-9.295	13.168	1.00	27.76
926	CA	GLN	A	606	13.916	-10.569	14	1.00	26.97
927	CB	GLN	A	606	13.579	-10.267	15.457	1.00	26.42
928	CD	GLN	A	606	13.176	-11.183	17.769	1.00	30.28
929	CG	GLN	A	606	13.372	-11.511	16.302	1.00	25.91
930	N	GLN	A	606	15.241	-11.191	13.902	1.00	25.48
931	NE2	GLN	A	606	14.088	-11.657	18.608	1.00	30.08
932	O	GLN	A	606	12.821	-9.033	12.504	1.00	26.77
933	OE1	GLN	A	606	12.22	-10.501	18.144	1.00	31.5
934	C	VAL	A	607	14.931	-7.63	10.928	1.00	25.23
935	CA	VAL	A	607	14.955	-7.281	12.425	1.00	26.21
936	CB	VAL	A	607	16.226	-6.467	12.785	1.00	28.94
937	CG1	VAL	A	607	16.379	-5.26	11.855	1.00	26.69
938	CG2	VAL	A	607	16.15	-6.009	14.244	1.00	25.03
939	N	VAL	A	607	14.895	-8.506	13.202	1.00	26.94
940	O	VAL	A	607	14.175	-7.036	10.158	1.00	25.66
941	C	ALA	A	608	14.38	-9.539	8.677	1.00	26.54
942	CA	ALA	A	608	15.768	-9.034	9.12	1.00	23.73
943	CB	ALA	A	608	16.819	-10.108	8.914	1.00	20.73

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FGFR1 COORDINATE DATA FOR RESIDUES 592-647

944	N	ALA	A	608	15.733	-8.612	10.522	1.00	25.45
945	O	ALA	A	608	13.969	-9.323	7.528	1.00	28.01
946	C	ARG	A	609	11.323	-9.546	9.115	1.00	25.47
947	CA	ARG	A	609	12.312	-10.689	9.292	1.00	28.73
948	CB	ARG	A	609	11.815	-11.61	10.391	1.00	31.51
949	CD	ARG	A	609	11.579	-13.892	11.099	1.00	40.28
950	CG	ARG	A	609	12.47	-12.94	10.386	1.00	35.36
951	CZ	ARG	A	609	10.045	-15.731	10.568	1.00	41.37
952	N	ARG	A	609	13.662	-10.2	9.585	1.00	27.79
953	NE	ARG	A	609	10.936	-14.822	10.186	1.00	41.71
954	NH1	ARG	A	609	9.686	-15.827	11.846	1.00	39.22
955	NH2	ARG	A	609	9.532	-16.562	9.674	1.00	41.27
956	O	ARG	A	609	10.464	-9.593	8.221	1.00	27.12
957	C	GLY	A	610	10.783	-6.741	8.521	1.00	25.53
958	CA	GLY	A	610	10.542	-7.389	9.88	1.00	22.03
959	N	GLY	A	610	11.405	-8.55	9.999	1.00	23.66
960	O	GLY	A	610	9.839	-6.422	7.781	1.00	23.51
961	C	MET	A	611	12.046	-6.868	5.701	1.00	23.88
962	CA	MET	A	611	12.447	-5.993	6.898	1.00	22.65
963	CB	MET	A	611	13.948	-5.722	6.868	1.00	21.92
964	CE	MET	A	611	13.818	-2.732	5.675	1.00	22.4
965	CG	MET	A	611	14.393	-4.549	7.738	1.00	22.8
966	N	MET	A	611	12.06	-6.584	8.175	1.00	23.11
967	O	MET	A	611	11.673	-6.36	4.646	1.00	24.59
968	SD	MET	A	611	13.487	-3.006	7.42	1.00	25.05
969	C	GLU	A	612	10.273	-8.852	4.435	1.00	26.04
970	CA	GLU	A	612	11.756	-9.066	4.775	1.00	25.56
971	CB	GLU	A	612	12.032	-10.517	5.156	1.00	25.06
972	CD	GLU	A	612	11.817	-12.941	4.457	1.00	26.78
973	CG	GLU	A	612	11.762	-11.497	4.02	1.00	26.17
974	N	GLU	A	612	12.123	-8.182	5.86	1.00	24.19
975	O	GLU	A	612	9.881	-8.805	3.261	1.00	24.7
976	OE1	GLU	A	612	11.521	-13.218	5.634	1.00	31.4
977	OE2	GLU	A	612	12.161	-13.809	3.624	1.00	31.87
978	C	TYR	A	613	7.792	-7.132	4.626	1.00	22.04
979	CA	TYR	A	613	8.029	-8.494	5.284	1.00	22.81
980	CB	TYR	A	613	7.315	-8.576	6.639	1.00	24.26
981	CD1	TYR	A	613	4.947	-9.228	6.109	1.00	21.44
982	CD2	TYR	A	613	5.364	-7	6.87	1.00	26.47
983	CE1	TYR	A	613	3.59	-8.944	5.988	1.00	21.03

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984	CE2	TYR	A	613	3.996	-6.698	6.746	1.00	24.75
985	CG	TYR	A	613	5.849	-8.266	6.549	1.00	23.29
986	CZ	TYR	A	613	3.126	-7.681	6.306	1.00	22.82
987	N	TYR	A	613	9.454	-8.72	5.47	1.00	23.73
988	O	TYR	A	613	7.012	-7.017	3.685	1.00	23.84
989	OH	TYR	A	613	1.793	-7.399	6.164	1.00	22.93
990	C	LEU	A	614	8.675	-4.67	3.113	1.00	23.93
991	CA	LEU	A	614	8.318	-4.745	4.607	1.00	22.45
992	CB	LEU	A	614	9.165	-3.762	5.424	1.00	21.56
993	CD1	LEU	A	614	9.537	-2.523	7.554	1.00	21.23
994	CD2	LEU	A	614	7.206	-2.665	6.586	1.00	22.41
995	CG	LEU	A	614	8.562	-3.387	6.782	1.00	24.95
996	N	LEU	A	614	8.444	-6.095	5.148	1.00	21.47
997	O	LEU	A	614	7.939	-4.078	2.314	1.00	24.61
998	C	ALA	A	615	9.193	-6.053	0.488	1.00	22.74
999	CA	ALA	A	615	10.228	-5.32	1.346	1.00	22.51
1000	CB	ALA	A	615	11.595	-6	1.231	1.00	22.19
1001	N	ALA	A	615	9.794	-5.287	2.737	1.00	23.78
1002	O	ALA	A	615	8.874	-5.59	-0.609	1.00	24.35
1003	C	SER	A	616	6.358	-7.118	0.031	1.00	24.48
1004	CA	SER	A	616	7.633	-7.939	0.281	1.00	22.68
1005	CB	SER	A	616	7.304	-9.23	1.033	1.00	21.53
1006	N	SER	A	616	8.641	-7.156	1.003	1.00	22.38
1007	O	SER	A	616	5.637	-7.332	-0.945	1.00	24.83
1008	OG	SER	A	616	6.41	-9.006	2.118	1.00	26.46
1009	C	LYS	A	617	5.34	-4.04	0.05	1.00	23.55
1010	CA	LYS	A	617	4.966	-5.291	0.829	1.00	22.27
1011	CB	LYS	A	617	4.466	-4.919	2.222	1.00	23.27
1012	CD	LYS	A	617	2.555	-6.497	2.203	1.00	31.19
1013	CE	LYS	A	617	1.817	-7.592	2.926	1.00	34.81
1014	CG	LYS	A	617	3.8	-6.075	2.948	1.00	26.96
1015	N	LYS	A	617	6.096	-6.178	0.931	1.00	23.69
1016	NZ	LYS	A	617	2.341	-8.928	2.585	1.00	43.88
1017	O	LYS	A	617	4.618	-3.044	0.089	1.00	24.37
1018	C	LYS	A	618	7.407	-1.696	-0.707	1.00	24.14
1019	CA	LYS	A	618	6.955	-2.957	-1.459	1.00	23.94
1020	CB	LYS	A	618	5.866	-2.596	-2.489	1.00	26.2
1021	CD	LYS	A	618	5.565	-4.944	-3.366	1.00	32.66
1022	CE	LYS	A	618	5.632	-5.828	-4.603	1.00	31.4
1023	CG	LYS	A	618	5.791	-3.494	-3.71	1.00	28.19

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1024	N	LYS	A	618	6.491	-4.072	-0.622	1.00	24.43
1025	NZ	LYS	A	618	4.369	-5.814	-5.375	1.00	36.63
1026	O	LYS	A	618	7.549	-0.615	-1.3	1.00	23.57
1027	C	CYS	A	619	9.631	-0.624	1.569	1.00	23.35
1028	CA	CYS	A	619	8.109	-0.733	1.418	1.00	26.09
1029	CB	CYS	A	619	7.451	-0.884	2.798	1.00	25.06
1030	N	CYS	A	619	7.698	-1.851	0.578	1.00	25.63
1031	O	CYS	A	619	10.303	-1.622	1.802	1.00	21.96
1032	SG	CYS	A	619	7.913	0.342	4.056	1.00	27.9
1033	C	ILE	A	620	11.625	1.757	2.753	1.00	24.6
1034	CA	ILE	A	620	11.598	0.86	1.511	1.00	24.21
1035	CB	ILE	A	620	12.202	1.64	0.274	1.00	24.98
1036	CD1	ILE	A	620	12.164	1.6	-2.293	1.00	25.87
1037	CG1	ILE	A	620	12.095	0.795	-0.999	1.00	23.97
1038	CG2	ILE	A	620	13.666	2.012	0.515	1.00	16.34
1039	N	ILE	A	620	10.166	0.576	1.349	1.00	23.25
1040	O	ILE	A	620	10.973	2.795	2.774	1.00	24.87
1041	C	HIS	A	621	13.072	3.413	4.912	1.00	26.24
1042	CA	HIS	A	621	12.417	2.057	5.06	1.00	25.37
1043	CB	HIS	A	621	13.183	1.252	6.133	1.00	22.77
1044	CD2	HIS	A	621	12.373	1.242	8.603	1.00	24.12
1045	CE1	HIS	A	621	13.079	3.23	9.189	1.00	25.7
1046	CG	HIS	A	621	13.002	1.772	7.536	1.00	26.47
1047	N	HIS	A	621	12.324	1.318	3.798	1.00	25.56
1048	ND1	HIS	A	621	13.439	3.03	7.939	1.00	26.62
1049	NE2	HIS	A	621	12.427	2.172	9.625	1.00	26.48
1050	O	HIS	A	621	12.514	4.421	5.331	1.00	25.7
1051	C	ARG	A	622	15.87	5.061	5.385	1.00	24.79
1052	CA	ARG	A	622	15.082	4.616	4.141	1.00	25.03
1053	CB	ARG	A	622	14.273	5.77	3.534	1.00	21.61
1054	CD	ARG	A	622	13.103	6.644	1.467	1.00	25.74
1055	CG	ARG	A	622	13.691	5.429	2.181	1.00	21.5
1056	CZ	ARG	A	622	11.592	5.549	-0.161	1.00	29.52
1057	N	ARG	A	622	14.269	3.416	4.336	1.00	25.55
1058	NE	ARG	A	622	12.683	6.267	0.114	1.00	27.69
1059	NH1	ARG	A	622	10.792	5.133	0.824	1.00	25.3
1060	NH2	ARG	A	622	11.328	5.199	-1.418	1.00	24.87
1061	O	ARG	A	622	16.784	5.856	5.28	1.00	25.5
1062	C	ASP	A	623	16.399	3.751	8.765	1.00	28.62
1063	CA	ASP	A	623	16.313	4.884	7.749	1.00	29.33

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1064	CB	ASP	A	623	15.8	6.168	8.409	1.00	32.72
1065	CG	ASP	A	623	16.764	6.705	9.478	1.00	37.45
1066	N	ASP	A	623	15.548	4.525	6.555	1.00	25.37
1067	O	ASP	A	623	16.11	3.927	9.954	1.00	27.4
1068	OD1	ASP	A	623	17.967	6.357	9.459	1.00	37.6
1069	OD2	ASP	A	623	16.309	7.467	10.354	1.00	44.55
1070	C	LEU	A	624	18.218	1.599	10.012	1.00	26.89
1071	CA	LEU	A	624	16.956	1.423	9.144	1.00	26.85
1072	CB	LEU	A	624	17.046	0.162	8.284	1.00	25.37
1073	CD1	LEU	A	624	15.857	-1.432	9.842	1.00	24.99
1074	CD2	LEU	A	624	17.319	-2.268	7.93	1.00	24.65
1075	CG	LEU	A	624	17.116	-1.188	8.988	1.00	24.54
1076	N	LEU	A	624	16.816	2.586	8.286	1.00	26.54
1077	O	LEU	A	624	19.334	1.753	9.501	1.00	28.27
1078	C	ALA	A	625	18.488	1.177	13.603	1.00	26.42
1079	CA	ALA	A	625	19.072	1.744	12.324	1.00	24.4
1080	CB	ALA	A	625	19.365	3.207	12.511	1.00	20.52
1081	N	ALA	A	625	18.016	1.575	11.325	1.00	27.62
1082	O	ALA	A	625	17.272	0.996	13.69	1.00	27.16
1083	C	ALA	A	626	17.914	1.361	16.574	1.00	25.56
1084	CA	ALA	A	626	18.851	0.37	15.868	1.00	24.58
1085	CB	ALA	A	626	20.024	0.002	16.785	1.00	24.02
1086	N	ALA	A	626	19.33	0.91	14.599	1.00	25.19
1087	O	ALA	A	626	17.043	0.952	17.33	1.00	27.72
1088	C	ARG	A	627	15.811	3.489	16.471	1.00	24.54
1089	CA	ARG	A	627	17.243	3.666	16.955	1.00	25.28
1090	CB	ARG	A	627	17.71	5.079	16.59	1.00	27.78
1091	CD	ARG	A	627	18.142	6.807	14.762	1.00	32.78
1092	CG	ARG	A	627	17.732	5.369	15.077	1.00	32.61
1093	CZ	ARG	A	627	19.643	6.864	12.802	1.00	36.7
1094	N	ARG	A	627	18.101	2.658	16.339	1.00	24.92
1095	NE	ARG	A	627	18.433	6.995	13.337	1.00	35.33
1096	NH1	ARG	A	627	20.684	6.557	13.565	1.00	40.06
1097	NH2	ARG	A	627	19.81	6.983	11.497	1.00	35.53
1098	O	ARG	A	627	14.871	3.855	17.163	1.00	23.65
1099	C	ASN	A	628	13.804	1.289	14.805	1.00	25.89
1100	CA	ASN	A	628	14.373	2.689	14.67	1.00	25.52
1101	CB	ASN	A	628	14.405	3.133	13.212	1.00	30.06
1102	CG	ASN	A	628	14.43	4.639	13.082	1.00	32.8
1103	N	ASN	A	628	15.668	2.911	15.283	1.00	24.28

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1104	ND2	ASN	A	628	15.239	5.143	12.173	1.00	35.27
1105	O	ASN	A	628	12.963	0.868	14.001	1.00	26.73
1106	OD1	ASN	A	628	13.765	5.341	13.836	1.00	34.62
1107	C	VAL	A	629	13.499	-0.667	17.604	1.00	27.53
1108	CA	VAL	A	629	13.848	-0.782	16.127	1.00	25.02
1109	CB	VAL	A	629	14.923	-1.88	15.957	1.00	26.46
1110	CG1	VAL	A	629	14.408	-3.201	16.565	1.00	21
1111	CG2	VAL	A	629	15.274	-2.07	14.456	1.00	22.93
1112	N	VAL	A	629	14.318	0.555	15.791	1.00	26.08
1113	O	VAL	A	629	14.333	-0.274	18.424	1.00	25.55
1114	C	LEU	A	630	11.632	-2.247	19.903	1.00	29.11
1115	CA	LEU	A	630	11.775	-0.85	19.298	1.00	29.9
1116	CB	LEU	A	630	10.459	-0.069	19.35	1.00	30.45
1117	CD1	LEU	A	630	9.105	1.973	18.76	1.00	28.2
1118	CD2	LEU	A	630	11.565	2.157	19.21	1.00	28.61
1119	CG	LEU	A	630	10.475	1.285	18.627	1.00	29.36
1120	N	LEU	A	630	12.243	-0.938	17.927	1.00	27.67
1121	O	LEU	A	630	11.398	-3.226	19.188	1.00	30.13
1122	C	VAL	A	631	10.537	-3.644	22.873	1.00	29.36
1123	CA	VAL	A	631	11.714	-3.621	21.902	1.00	27.16
1124	CB	VAL	A	631	13.046	-3.912	22.668	1.00	29.12
1125	CG1	VAL	A	631	13.058	-5.339	23.202	1.00	21.33
1126	CG2	VAL	A	631	14.252	-3.66	21.757	1.00	25.9
1127	N	VAL	A	631	11.793	-2.341	21.219	1.00	28.87
1128	O	VAL	A	631	10.37	-2.739	23.702	1.00	29.44
1129	C	THR	A	632	8.895	-5.488	24.94	1.00	34.68
1130	CA	THR	A	632	8.542	-4.84	23.603	1.00	32.49
1131	CB	THR	A	632	7.469	-5.686	22.882	1.00	31.46
1132	CG2	THR	A	632	7.275	-5.17	21.458	1.00	27.43
1133	N	THR	A	632	9.717	-4.68	22.755	1.00	30.9
1134	O	THR	A	632	10.008	-5.981	25.115	1.00	35.81
1135	OG1	THR	A	632	7.878	-7.064	22.835	1.00	31.69
1136	C	GLU	A	633	8.597	-7.566	27.05	1.00	36.96
1137	CA	GLU	A	633	8.144	-6.119	27.183	1.00	37.24
1138	CB	GLU	A	633	6.856	-6.048	28.009	1.00	38.36
1139	CD	GLU	A	633	8.061	-6.006	30.297	1.00	49.87
1140	CG	GLU	A	633	6.958	-6.636	29.428	1.00	45.94
1141	N	GLU	A	633	7.938	-5.511	25.868	1.00	37.03
1142	O	GLU	A	633	9.329	-8.066	27.892	1.00	38.37
1143	OE1	GLU	A	633	8.173	-4.759	30.346	1.00	50.93

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TABLE 9  
FGFR1 COORDINATE DATA FOR RESIDUES 592-647

1144	OE2	GLU	A	633	8.812	-6.768	30.952	1.00	52.11
1145	C	ASP	A	634	9.835	-9.765	24.91	1.00	37.04
1146	CA	ASP	A	634	8.558	-9.62	25.741	1.00	38.95
1147	CB	ASP	A	634	7.424	-10.375	25.035	1.00	44.26
1148	CG	ASP	A	634	6.064	-10.141	25.678	1.00	51.87
1149	N	ASP	A	634	8.187	-8.225	25.971	1.00	38.2
1150	O	ASP	A	634	10.138	-10.859	24.447	1.00	37.11
1151	OD1	ASP	A	634	5.898	-10.452	26.877	1.00	53.17
1152	OD2	ASP	A	634	5.155	-9.647	24.975	1.00	57.57
1153	C	ASN	A	635	11.629	-8.979	22.448	1.00	34.75
1154	CA	ASN	A	635	11.826	-8.662	23.939	1.00	36.9
1155	CB	ASN	A	635	12.882	-9.609	24.532	1.00	36.1
1156	CG	ASN	A	635	13.221	-9.275	25.965	1.00	36.16
1157	N	ASN	A	635	10.58	-8.674	24.736	1.00	36.81
1158	ND2	ASN	A	635	13.447	-10.299	26.766	1.00	39.38
1159	O	ASN	A	635	12.429	-9.695	21.836	1.00	33.92
1160	OD1	ASN	A	635	13.251	-8.113	26.354	1.00	37.91
1161	C	VAL	A	636	10.756	-7.445	19.774	1.00	27.35
1162	CA	VAL	A	636	10.283	-8.71	20.465	1.00	29.36
1163	CB	VAL	A	636	8.788	-8.969	20.177	1.00	29.98
1164	CG1	VAL	A	636	8.554	-9.13	18.671	1.00	29.92
1165	CG2	VAL	A	636	8.339	-10.23	20.899	1.00	28.04
1166	N	VAL	A	636	10.537	-8.487	21.874	1.00	31.68
1167	O	VAL	A	636	10.478	-6.347	20.236	1.00	25.37
1168	C	MET	A	637	11.028	-6.085	16.99	1.00	24.43
1169	CA	MET	A	637	12.108	-6.498	17.977	1.00	25.59
1170	CB	MET	A	637	13.351	-6.938	17.199	1.00	27.32
1171	CE	MET	A	637	15.101	-7.464	20.682	1.00	27.65
1172	CG	MET	A	637	14.458	-7.552	18.044	1.00	29.53
1173	N	MET	A	637	11.573	-7.616	18.74	1.00	27.82
1174	O	MET	A	637	10.473	-6.928	16.297	1.00	24.82
1175	SD	MET	A	637	15.12	-6.414	19.286	1.00	29.77
1176	C	LYS	A	638	10.261	-3.053	15.285	1.00	24.97
1177	CA	LYS	A	638	9.735	-4.265	16.018	1.00	23.94
1178	CB	LYS	A	638	8.471	-3.889	16.781	1.00	21.9
1179	CD	LYS	A	638	6.4	-4.684	18.019	1.00	24.28
1180	CE	LYS	A	638	5.482	-5.899	18.273	1.00	23.43
1181	CG	LYS	A	638	7.704	-5.09	17.306	1.00	24.53
1182	N	LYS	A	638	10.743	-4.791	16.923	1.00	25.58
1183	NZ	LYS	A	638	4.861	-6.398	17	1.00	24.81

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TABLE 9  
FGFR1 COORDINATE DATA FOR RESIDUES 592-647

1184	O	LYS	A	638	10.687	-2.084	15.899	1.00	26.96
1185	C	ILE	A	639	9.661	-0.895	13.233	1.00	27.2
1186	CA	ILE	A	639	10.708	-2.006	13.142	1.00	26.32
1187	CB	ILE	A	639	10.927	-2.449	11.656	1.00	27.24
1188	CD1	ILE	A	639	12.128	-4.208	10.322	1.00	33.01
1189	CG1	ILE	A	639	12.087	-3.45	11.591	1.00	27.89
1190	CG2	ILE	A	639	11.231	-1.239	10.755	1.00	21.86
1191	N	ILE	A	639	10.254	-3.119	13.963	1.00	26.37
1192	O	ILE	A	639	8.453	-1.139	13.093	1.00	24.78
1193	C	ALA	A	640	9.642	2.519	12.535	1.00	27.14
1194	CA	ALA	A	640	9.318	1.5	13.623	1.00	27.15
1195	CB	ALA	A	640	9.562	2.121	14.998	1.00	25.59
1196	N	ALA	A	640	10.147	0.316	13.485	1.00	27.6
1197	O	ALA	A	640	10.695	2.448	11.892	1.00	27.26
1198	C	ASP	A	641	9.063	4.123	9.904	1.00	30.46
1199	CA	ASP	A	641	8.877	4.543	11.35	1.00	31.13
1200	CB	ASP	A	641	10.021	5.487	11.748	1.00	34.1
1201	CG	ASP	A	641	9.713	6.309	12.994	1.00	37.62
1202	N	ASP	A	641	8.721	3.453	12.324	1.00	27.7
1203	O	ASP	A	641	9.605	4.881	9.105	1.00	30.84
1204	OD1	ASP	A	641	8.718	6.026	13.678	1.00	34.58
1205	OD2	ASP	A	641	10.49	7.24	13.302	1.00	43.02
1206	C	PHE	A	642	7.757	3.137	7.204	1.00	33.72
1207	CA	PHE	A	642	8.694	2.43	8.197	1.00	30.93
1208	CB	PHE	A	642	8.48	0.909	8.168	1.00	26.43
1209	CD1	PHE	A	642	5.995	0.485	7.99	1.00	27.62
1210	CD2	PHE	A	642	7.098	0.022	10.069	1.00	26.65
1211	CE1	PHE	A	642	4.767	0.075	8.534	1.00	25.93
1212	CE2	PHE	A	642	5.88	-0.388	10.627	1.00	27.61
1213	CG	PHE	A	642	7.167	0.463	8.755	1.00	27.46
1214	CZ	PHE	A	642	4.712	-0.364	9.856	1.00	28.77
1215	N	PHE	A	642	8.58	2.935	9.56	1.00	30.42
1216	O	PHE	A	642	8.033	3.163	5.998	1.00	36.04
1217	C	GLY	A	643	5.823	5.927	6.911	1.00	32.91
1218	CA	GLY	A	643	5.735	4.421	6.841	1.00	31.57
1219	N	GLY	A	643	6.687	3.748	7.712	1.00	32.87
1220	O	GLY	A	643	4.961	6.643	6.408	1.00	33.29
1221	C	LEU	A	644	7.286	8.576	6.355	1.00	41.96
1222	CA	LEU	A	644	7.156	7.817	7.675	1.00	38.87
1223	CB	LEU	A	644	8.415	8.001	8.51	1.00	38.36



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TABLE 9

## FGFR1 COORDINATE DATA FOR RESIDUES 592-647

1224	CD1	LEU	A	644	7.273	8.875	10.536	1.00	45.11
1225	CD2	LEU	A	644	9.759	9.189	10.238	1.00	44.92
1226	CG	LEU	A	644	8.399	9.124	9.533	1.00	43.07
1227	N	LEU	A	644	6.91	6.401	7.497	1.00	35.46
1228	O	LEU	A	644	7.93	8.114	5.407	1.00	43.84
1229	C	ALA	A	645	7.97	11.412	5.202	1.00	45.04
1230	CA	ALA	A	645	6.694	10.577	5.108	1.00	45.17
1231	CB	ALA	A	645	5.466	11.482	5.076	1.00	44.97
1232	N	ALA	A	645	6.649	9.736	6.293	1.00	43.68
1233	O	ALA	A	645	8.234	12.044	6.225	1.00	44.74
1234	C	ARG	A	646	10.453	12.562	2.765	1.00	46.86
1235	CA	ARG	A	646	10.018	12.155	4.158	1.00	46.9
1236	CB	ARG	A	646	11.141	11.342	4.809	1.00	48.15
1237	N	ARG	A	646	8.775	11.394	4.151	1.00	44.59
1238	O	ARG	A	646	10.407	11.757	1.837	1.00	45.75
1239	C	ASP	A	647	12.829	14.123	1.378	1.00	51.45
1240	CA	ASP	A	647	11.323	14.294	1.32	1.00	51.43
1241	CB	ASP	A	647	10.969	15.761	1.088	1.00	52.64
1242	CG	ASP	A	647	11.199	16.201	-0.356	1.00	55.88
1243	N	ASP	A	647	10.846	13.823	2.612	1.00	49.41
1244	O	ASP	A	647	13.516	14.817	2.136	1.00	48.94
1245	OD1	ASP	A	647	12.244	15.852	-0.963	1.00	51.91
1246	OD2	ASP	A	647	10.318	16.914	-0.886	1.00	59.87

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TABLE 10  
FGFR1 COORDINATE DATA FOR RESIDUES 651-761

ATOM	ATOM TYPE	RESIDUE	PROTEIN #	#	X	Y	Z	OCC	B
1275	C	ILE	A	651	18.514	16.71	4.553	1.00	60.6
1276	CA	ILE	A	651	17.294	15.879	4.185	1.00	61.74
1277	CB	ILE	A	651	17.732	14.407	4.002	1.00	63.76
1278	CD1	ILE	A	651	16.83	12.04	3.711	1.00	66.12
1279	CG1	ILE	A	651	16.507	13.503	3.95	1.00	65.01
1280	CG2	ILE	A	651	18.665	13.976	5.143	1.00	62.99
1281	N	ILE	A	651	16.67	16.392	2.977	1.00	63.1
1282	O	ILE	A	651	19.375	16.958	3.719	1.00	60.84
1283	C	ASP	A	652	20.769	16.935	6.681	1.00	56.79
1284	CA	ASP	A	652	19.692	17.932	6.273	1.00	58.25
1285	CB	ASP	A	652	19.28	18.772	7.484	1.00	59.79
1286	CG	ASP	A	652	20.461	19.508	8.139	1.00	62.27
1287	N	ASP	A	652	18.564	17.16	5.797	1.00	59.57
1288	O	ASP	A	652	20.671	16.308	7.736	1.00	56.21
1289	OD1	ASP	A	652	21.486	19.756	7.472	1.00	63.25
1290	OD2	ASP	A	652	20.324	19.84	9.326	1.00	63.49
1291	C	TYR	A	653	23.7	16.167	7.346	1.00	55.65
1292	CA	TYR	A	653	22.89	15.864	6.092	1.00	54.73
1293	CB	TYR	A	653	23.82	15.816	4.879	1.00	53.42
1294	CD1	TYR	A	653	22.115	14.223	3.919	1.00	53.39
1295	CD2	TYR	A	653	24.132	14.605	2.684	1.00	51.68
1296	CE1	TYR	A	653	21.685	13.313	2.961	1.00	54.75
1297	CE2	TYR	A	653	23.714	13.699	1.715	1.00	53.43
1298	CG	TYR	A	653	23.343	14.878	3.8	1.00	52.69
1299	CZ	TYR	A	653	22.486	13.053	1.86	1.00	54.53
1300	N	TYR	A	653	21.782	16.784	5.836	1.00	55.55
1301	O	TYR	A	653	24.351	15.283	7.909	1.00	54.58
1302	OH	TYR	A	653	22.064	12.146	0.913	1.00	53.59
1303	C	TYR	A	654	23.614	17.725	10.245	1.00	59.79
1304	CA	TYR	A	654	24.417	17.823	8.954	1.00	58.48
1305	CB	TYR	A	654	24.973	19.231	8.742	1.00	57.63
1306	CD1	TYR	A	654	25.743	19.357	6.33	1.00	60.91
1307	CD2	TYR	A	654	27.403	19.195	8.045	1.00	61.19
1308	CE1	TYR	A	654	26.743	19.362	5.356	1.00	62.94
1309	CE2	TYR	A	654	28.408	19.2	7.084	1.00	63.46
1310	CG	TYR	A	654	26.058	19.272	7.687	1.00	59.98
1311	CZ	TYR	A	654	28.077	19.284	5.743	1.00	64.35
1312	N	TYR	A	654	23.669	17.419	7.777	1.00	56.62

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TABLE 10  
FGFR1 COORDINATE DATA FOR RESIDUES 651-761

1313	O	TYR	A	654	24.15	17.946	11.33	1.00	60.6
1314	OH	TYR	A	654	29.083	19.295	4.798	1.00	63.43
1315	C	LYS	A	655	21.767	15.934	12.052	1.00	61.97
1316	CA	LYS	A	655	21.485	17.224	11.294	1.00	61.83
1317	CB	LYS	A	655	20.011	17.281	10.888	1.00	63.91
1318	CD	LYS	A	655	17.645	17.656	11.547	1.00	73.08
1319	CE	LYS	A	655	16.579	17.244	12.544	1.00	77.19
1320	CG	LYS	A	655	19.038	17.328	12.048	1.00	67.08
1321	N	LYS	A	655	22.345	17.346	10.129	1.00	60.28
1322	NZ	LYS	A	655	15.204	17.494	12.014	1.00	80.81
1323	O	LYS	A	655	21.955	14.873	11.454	1.00	61.35
1324	C	LYS	A	656	20.781	14.332	14.802	1.00	61.61
1325	CA	LYS	A	656	22.071	14.899	14.232	1.00	62.12
1326	CB	LYS	A	656	23.019	15.287	15.37	1.00	62.28
1327	CD	LYS	A	656	25.292	15.913	16.164	1.00	66.44
1328	CE	LYS	A	656	26.782	15.727	15.93	1.00	67.32
1329	CG	LYS	A	656	24.466	15.479	14.966	1.00	63.18
1330	N	LYS	A	656	21.812	16.042	13.375	1.00	61.96
1331	NZ	LYS	A	656	27.577	16.103	17.136	1.00	67.82
1332	O	LYS	A	656	19.71	14.939	14.687	1.00	62.39
1333	C	THR	A	657	19.64	13.072	17.435	1.00	57.49
1334	CA	THR	A	657	19.751	12.493	16.03	1.00	57.35
1335	CB	THR	A	657	20.008	10.969	16.127	1.00	55.72
1336	CG2	THR	A	657	20.272	10.379	14.755	1.00	52.32
1337	N	THR	A	657	20.889	13.157	15.41	1.00	59.7
1338	O	THR	A	657	20.452	13.912	17.821	1.00	57.58
1339	OG1	THR	A	657	21.144	10.715	16.97	1.00	55.11
1340	C	THR	A	658	19.759	12.777	20.373	1.00	60.17
1341	CA	THR	A	658	18.514	13.126	19.573	1.00	59.99
1342	CB	THR	A	658	17.277	12.517	20.291	1.00	60.58
1343	N	THR	A	658	18.66	12.623	18.209	1.00	58.48
1344	O	THR	A	658	20.259	13.6	21.137	1.00	60.05
1345	C	ASN	A	659	22.754	11.762	20.3	1.00	56.94
1346	CA	ASN	A	659	21.486	11.093	20.817	1.00	58.3
1347	CB	ASN	A	659	21.61	9.579	20.656	1.00	60.25
1348	CG	ASN	A	659	22.423	8.94	21.766	1.00	60.93
1349	N	ASN	A	659	20.291	11.578	20.129	1.00	59.82
1350	ND2	ASN	A	659	23.154	7.882	21.435	1.00	57.59
1351	O	ASN	A	659	23.842	11.481	20.787	1.00	56.52

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TABLE 10  
FGFR1 COORDINATE DATA FOR RESIDUES 651-761

1352	OD1	ASN	A	659	22.369	9.378	22.916	1.00	62.61
1353	C	GLY	A	660	24.526	12.588	17.643	1.00	53.32
1354	CA	GLY	A	660	23.738	13.319	18.714	1.00	54.97
1355	N	GLY	A	660	22.606	12.61	19.285	1.00	56.43
1356	O	GLY	A	660	25.727	12.825	17.484	1.00	54.63
1357	C	ARG	A	661	24.081	11.416	14.474	1.00	46.96
1358	CA	ARG	A	661	24.543	10.947	15.849	1.00	49.14
1359	CB	ARG	A	661	24.285	9.446	15.985	1.00	48.09
1360	CD	ARG	A	661	24.548	7.306	17.202	1.00	50
1361	CG	ARG	A	661	24.815	8.802	17.254	1.00	49.27
1362	CZ	ARG	A	661	24.912	5.269	18.534	1.00	48.92
1363	N	ARG	A	661	23.868	11.701	16.906	1.00	51.74
1364	NE	ARG	A	661	25.036	6.583	18.373	1.00	48.78
1365	NH1	ARG	A	661	24.312	4.542	17.595	1.00	45.08
1366	NH2	ARG	A	661	25.405	4.682	19.622	1.00	46.99
1367	O	ARG	A	661	23.01	12.007	14.336	1.00	45.17
1368	C	LEU	A	662	23.966	10.371	11.285	1.00	39.21
1369	CA	LEU	A	662	24.569	11.517	12.097	1.00	41.36
1370	CB	LEU	A	662	25.836	12.035	11.404	1.00	40.81
1371	CD1	LEU	A	662	27.882	13.494	11.569	1.00	41.46
1372	CD2	LEU	A	662	25.59	14.522	11.496	1.00	41.61
1373	CG	LEU	A	662	26.421	13.336	11.966	1.00	43.48
1374	N	LEU	A	662	24.883	11.119	13.46	1.00	43.26
1375	O	LEU	A	662	24.669	9.443	10.896	1.00	37.92
1376	C	PRO	A	663	22.57	9.061	8.889	1.00	33.24
1377	CA	PRO	A	663	21.914	9.427	10.228	1.00	35.69
1378	CB	PRO	A	663	20.547	10.087	10.024	1.00	36.3
1379	CD	PRO	A	663	21.742	11.48	11.507	1.00	38.44
1380	CG	PRO	A	663	20.372	10.853	11.308	1.00	40.16
1381	N	PRO	A	663	22.653	10.436	11.002	1.00	37.47
1382	O	PRO	A	663	22.386	7.947	8.388	1.00	31.81
1383	C	VAL	A	664	24.958	8.479	7.177	1.00	29.99
1384	CA	VAL	A	664	24.022	9.68	7.045	1.00	32.49
1385	CB	VAL	A	664	24.832	10.885	6.473	1.00	32.61
1386	CG1	VAL	A	664	23.893	11.89	5.853	1.00	33.49
1387	CG2	VAL	A	664	25.682	11.532	7.555	1.00	33.4
1388	N	VAL	A	664	23.348	9.977	8.316	1.00	32.12
1389	O	VAL	A	664	25.307	7.866	6.18	1.00	27.24
1390	C	LYS	A	665	25.555	5.65	8.465	1.00	26.69

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TABLE 10  
FGFR1 COORDINATE DATA FOR RESIDUES 651-761

1391	CA	LYS	A	665	26.198	7.004	8.682	1.00	27.82
1392	CB	LYS	A	665	26.82	7.119	10.072	1.00	26.97
1393	CD	LYS	A	665	28.302	8.597	11.486	1.00	30.95
1394	CE	LYS	A	665	29.552	9.476	11.448	1.00	31.3
1395	CG	LYS	A	665	27.971	8.102	10.088	1.00	29.53
1396	N	LYS	A	665	25.319	8.13	8.414	1.00	28.84
1397	NZ	LYS	A	665	29.843	10.164	12.742	1.00	32.56
1398	O	LYS	A	665	26.226	4.629	8.558	1.00	26.68
1399	C	TRP	A	666	23.191	4.281	6.387	1.00	23.63
1400	CA	TRP	A	666	23.554	4.403	7.871	1.00	26.2
1401	CB	TRP	A	666	22.288	4.287	8.73	1.00	25.03
1402	CD1	TRP	A	666	22.357	2.636	10.716	1.00	20.31
1403	CD2	TRP	A	666	23.048	4.708	11.232	1.00	24.35
1404	CE2	TRP	A	666	23.124	3.902	12.391	1.00	24.14
1405	CE3	TRP	A	666	23.432	6.052	11.313	1.00	23.93
1406	CG	TRP	A	666	22.554	3.873	10.17	1.00	26.48
1407	CH2	TRP	A	666	23.941	5.724	13.673	1.00	26.02
1408	CZ2	TRP	A	666	23.57	4.402	13.624	1.00	25.24
1409	CZ3	TRP	A	666	23.876	6.547	12.538	1.00	25.72
1410	N	TRP	A	666	24.263	5.645	8.153	1.00	25.87
1411	NE1	TRP	A	666	22.702	2.648	12.045	1.00	22.04
1412	O	TRP	A	666	22.803	3.215	5.927	1.00	24.75
1413	C	MET	A	667	23.982	4.695	3.234	1.00	22.71
1414	CA	MET	A	667	23.041	5.373	4.209	1.00	24.22
1415	CB	MET	A	667	22.906	6.814	3.737	1.00	26.48
1416	CE	MET	A	667	21.019	8.954	2.239	1.00	41.11
1417	CG	MET	A	667	21.846	7.626	4.43	1.00	35.64
1418	N	MET	A	667	23.396	5.349	5.628	1.00	22.85
1419	O	MET	A	667	25.2	4.88	3.297	1.00	23.89
1420	SD	MET	A	667	21.815	9.287	3.722	1.00	42.33
1421	C	ALA	A	668	24.807	4.487	0.431	1.00	25.51
1422	CA	ALA	A	668	24.205	3.339	1.232	1.00	23.61
1423	CB	ALA	A	668	23.336	2.496	0.332	1.00	22.02
1424	N	ALA	A	668	23.407	3.972	2.274	1.00	22.28
1425	O	ALA	A	668	24.195	5.553	0.314	1.00	23.93
1426	C	PRO	A	669	25.662	5.895	-2.055	1.00	26.45
1427	CA	PRO	A	669	26.588	5.375	-0.943	1.00	27.66
1428	CB	PRO	A	669	27.852	4.742	-1.516	1.00	25.35
1429	CD	PRO	A	669	26.888	3.114	-0.13	1.00	25.53

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1430	CG	PRO	A	669	28.209	3.729	-0.475	1.00	24.07
1431	N	PRO	A	669	25.994	4.283	-0.163	1.00	27.09
1432	O	PRO	A	669	25.589	7.102	-2.275	1.00	28.1
1433	C	GLU	A	670	22.84	6.278	-3.285	1.00	27.86
1434	CA	GLU	A	670	24.036	5.458	-3.797	1.00	28.64
1435	CB	GLU	A	670	23.572	4.292	-4.693	1.00	31.17
1436	CD	GLU	A	670	23.231	2.185	-3.266	1.00	32.87
1437	CG	GLU	A	670	22.615	3.31	-4.011	1.00	32.16
1438	N	GLU	A	670	24.93	5.006	-2.726	1.00	26.68
1439	O	GLU	A	670	22.348	7.171	-3.977	1.00	24.91
1440	OE1	GLU	A	670	24.453	2.14	-3.107	1.00	29.23
1441	OE2	GLU	A	670	22.471	1.321	-2.816	1.00	24.81
1442	C	ALA	A	671	21.886	8.111	-0.984	1.00	30.95
1443	CA	ALA	A	671	21.331	6.766	-1.436	1.00	30.35
1444	CB	ALA	A	671	20.744	6	-0.256	1.00	25.16
1445	N	ALA	A	671	22.427	6.02	-2.046	1.00	29.44
1446	O	ALA	A	671	21.291	9.152	-1.23	1.00	32.76
1447	C	LEU	A	672	24.167	10.188	-1.021	1.00	36.29
1448	CA	LEU	A	672	23.715	9.285	0.115	1.00	33.73
1449	CB	LEU	A	672	24.919	8.915	0.967	1.00	34.39
1450	CD1	LEU	A	672	25.013	10.825	2.572	1.00	40.69
1451	CD2	LEU	A	672	27.047	9.518	2.069	1.00	33.28
1452	CG	LEU	A	672	25.765	10.07	1.493	1.00	37.98
1453	N	LEU	A	672	23.061	8.081	-0.369	1.00	32.63
1454	O	LEU	A	672	23.804	11.354	-1.069	1.00	37.84
1455	C	PHE	A	673	24.507	10.664	-4.197	1.00	36.1
1456	CA	PHE	A	673	25.48	10.419	-3.054	1.00	35.27
1457	CB	PHE	A	673	26.743	9.757	-3.613	1.00	34.5
1458	CD1	PHE	A	673	28.243	10.692	-1.816	1.00	36.6
1459	CD2	PHE	A	673	28.535	8.41	-2.489	1.00	32.81
1460	CE1	PHE	A	673	29.304	10.563	-0.897	1.00	39.12
1461	CE2	PHE	A	673	29.593	8.269	-1.577	1.00	37.16
1462	CG	PHE	A	673	27.856	9.616	-2.615	1.00	33.68
1463	CZ	PHE	A	673	29.979	9.346	-0.781	1.00	36.22
1464	N	PHE	A	673	24.965	9.648	-1.935	1.00	35.17
1465	O	PHE	A	673	24.48	11.752	-4.759	1.00	36.81
1466	C	ASP	A	674	21.305	9.836	-5.35	1.00	40.56
1467	CA	ASP	A	674	22.79	9.769	-5.669	1.00	38.32
1468	CB	ASP	A	674	23.039	8.612	-6.636	1.00	40.57

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1469	CG	ASP	A	674	24.476	8.553	-7.113	1.00	43.96
1470	N	ASP	A	674	23.708	9.66	-4.542	1.00	38.14
1471	O	ASP	A	674	20.473	9.849	-6.272	1.00	39.62
1472	OD1	ASP	A	674	25.107	9.627	-7.237	1.00	43.49
1473	OD2	ASP	A	674	24.977	7.429	-7.348	1.00	48.12
1474	C	ARG	A	675	18.715	8.779	-4.233	1.00	38.76
1475	CA	ARG	A	675	19.568	9.903	-3.641	1.00	42.16
1476	CB	ARG	A	675	18.975	11.274	-3.969	1.00	48.49
1477	CD	ARG	A	675	19.654	13.69	-4.059	1.00	68.79
1478	CG	ARG	A	675	19.655	12.415	-3.227	1.00	59.57
1479	CZ	ARG	A	675	19.776	16.082	-3.464	1.00	80.12
1480	N	ARG	A	675	20.965	9.843	-4.064	1.00	40.27
1481	NE	ARG	A	675	20.193	14.827	-3.315	1.00	76.31
1482	NH1	ARG	A	675	18.812	16.374	-4.336	1.00	81.6
1483	NH2	ARG	A	675	20.316	17.049	-2.731	1.00	82.67
1484	O	ARG	A	675	17.527	8.948	-4.512	1.00	39.05
1485	C	ILE	A	676	18.384	5.498	-3.819	1.00	30.88
1486	CA	ILE	A	676	18.619	6.485	-4.961	1.00	33.29
1487	CB	ILE	A	676	19.412	5.806	-6.067	1.00	33.79
1488	CD1	ILE	A	676	20.837	6.321	-8.118	1.00	40.54
1489	CG1	ILE	A	676	19.785	6.825	-7.146	1.00	36.84
1490	CG2	ILE	A	676	18.582	4.701	-6.662	1.00	33.81
1491	N	ILE	A	676	19.331	7.626	-4.431	1.00	35.15
1492	O	ILE	A	676	19.323	4.894	-3.297	1.00	28.54
1493	C	TYR	A	677	16.046	3.228	-2.909	1.00	22.97
1494	CA	TYR	A	677	16.711	4.464	-2.349	1.00	25.81
1495	CB	TYR	A	677	15.763	5.193	-1.404	1.00	26.35
1496	CD1	TYR	A	677	16.645	7.528	-0.984	1.00	27.45
1497	CD2	TYR	A	677	16.935	5.867	0.722	1.00	24.65
1498	CE1	TYR	A	677	17.26	8.471	-0.177	1.00	26.76
1499	CE2	TYR	A	677	17.544	6.805	1.536	1.00	26.12
1500	CG	TYR	A	677	16.469	6.212	-0.546	1.00	27.17
1501	CZ	TYR	A	677	17.7	8.1	1.087	1.00	28.9
1502	N	TYR	A	677	17.121	5.357	-3.43	1.00	30.18
1503	O	TYR	A	677	15.163	3.325	-3.758	1.00	26.54
1504	OH	TYR	A	677	18.255	9.03	1.936	1.00	35.99
1505	C	THR	A	678	15.996	-0.182	-1.7	1.00	22.75
1506	CA	THR	A	678	15.961	0.787	-2.87	1.00	22.1
1507	CB	THR	A	678	16.906	0.192	-3.931	1.00	23.87

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1508	CG2	THR	A	678	16.912	1.033	-5.205	1.00	24.19
1509	N	THR	A	678	16.464	2.068	-2.416	1.00	21.87
1510	O	THR	A	678	16.431	0.159	-0.596	1.00	23.41
1511	OG1	THR	A	678	18.236	0.159	-3.387	1.00	27.47
1512	C	HIS	A	679	17.099	-2.709	-0.661	1.00	23.16
1513	CA	HIS	A	679	15.616	-2.415	-0.901	1.00	23.19
1514	CB	HIS	A	679	14.872	-3.677	-1.346	1.00	22.26
1515	CD2	HIS	A	679	12.707	-3.569	-2.778	1.00	26.22
1516	CE1	HIS	A	679	11.337	-2.845	-1.22	1.00	28.48
1517	CG	HIS	A	679	13.416	-3.445	-1.626	1.00	25.39
1518	N	HIS	A	679	15.566	-1.407	-1.944	1.00	21.87
1519	ND1	HIS	A	679	12.533	-2.998	-0.676	1.00	26.46
1520	NE2	HIS	A	679	11.417	-3.183	-2.491	1.00	29.57
1521	O	HIS	A	679	17.51	-3.039	0.457	1.00	22.43
1522	C	GLN	A	680	20.007	-1.751	-0.734	1.00	22.87
1523	CA	GLN	A	680	19.343	-2.739	-1.667	1.00	22.07
1524	CB	GLN	A	680	19.962	-2.592	-3.064	1.00	22.39
1525	CD	GLN	A	680	18.859	-3.86	-4.983	1.00	33.96
1526	CG	GLN	A	680	19.923	-3.858	-3.902	1.00	28.94
1527	N	GLN	A	680	17.9	-2.52	-1.711	1.00	22.37
1528	NE2	GLN	A	680	19.098	-4.624	-6.045	1.00	32.65
1529	O	GLN	A	680	20.935	-2.107	-0.011	1.00	22.23
1530	OE1	GLN	A	680	17.812	-3.226	-4.844	1.00	38.45
1531	C	SER	A	681	19.776	0.199	1.576	1.00	22.91
1532	CA	SER	A	681	20.184	0.471	0.128	1.00	23.64
1533	CB	SER	A	681	19.905	1.918	-0.316	1.00	20.82
1534	N	SER	A	681	19.57	-0.498	-0.761	1.00	22.4
1535	O	SER	A	681	20.533	0.518	2.497	1.00	24.18
1536	OG	SER	A	681	18.525	2.197	-0.479	1.00	23.33
1537	C	ASP	A	682	18.977	-1.897	3.692	1.00	20.42
1538	CA	ASP	A	682	18.112	-0.783	3.104	1.00	22.02
1539	CB	ASP	A	682	16.661	-1.273	3.029	1.00	24.79
1540	CG	ASP	A	682	15.63	-0.16	3.22	1.00	24.36
1541	N	ASP	A	682	18.608	-0.425	1.765	1.00	22.95
1542	O	ASP	A	682	19.155	-1.997	4.909	1.00	21.66
1543	OD1	ASP	A	682	15.98	0.985	3.589	1.00	24.8
1544	OD2	ASP	A	682	14.437	-0.461	3.025	1.00	25.32
1545	C	VAL	A	683	21.671	-3.321	3.685	1.00	19.72
1546	CA	VAL	A	683	20.332	-3.872	3.181	1.00	20.04



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1547	CB	VAL	A	683	20.488	-4.853	2	1.00	22.27
1548	CG1	VAL	A	683	21.738	-5.714	2.166	1.00	19.23
1549	CG2	VAL	A	683	19.244	-5.73	1.915	1.00	22.21
1550	N	VAL	A	683	19.474	-2.759	2.808	1.00	19.45
1551	O	VAL	A	683	22.201	-3.79	4.682	1.00	21.1
1552	C	TRP	A	684	23.191	-1.183	4.899	1.00	23.41
1553	CA	TRP	A	684	23.437	-1.671	3.452	1.00	22.38
1554	CB	TRP	A	684	23.769	-0.484	2.534	1.00	18.73
1555	CD1	TRP	A	684	24.928	1.215	4.111	1.00	22.57
1556	CD2	TRP	A	684	26.231	0.463	2.453	1.00	24.39
1557	CE2	TRP	A	684	26.986	1.36	3.257	1.00	25.01
1558	CE3	TRP	A	684	26.849	-0.133	1.341	1.00	24.48
1559	CG	TRP	A	684	24.921	0.383	3.02	1.00	22.66
1560	CH2	TRP	A	684	28.905	1.07	1.889	1.00	24.3
1561	CZ2	TRP	A	684	28.322	1.668	2.984	1.00	25.05
1562	CZ3	TRP	A	684	28.189	0.182	1.069	1.00	24.44
1563	N	TRP	A	684	22.208	-2.319	3.002	1.00	20.82
1564	NE1	TRP	A	684	26.166	1.804	4.262	1.00	23.32
1565	O	TRP	A	684	23.971	-1.485	5.811	1.00	24.28
1566	C	SER	A	685	21.663	-1.079	7.455	1.00	23.66
1567	CA	SER	A	685	21.736	0.067	6.439	1.00	23.99
1568	CB	SER	A	685	20.371	0.756	6.387	1.00	22.18
1569	N	SER	A	685	22.104	-0.438	5.108	1.00	23.11
1570	O	SER	A	685	22.091	-0.927	8.609	1.00	23.59
1571	OG	SER	A	685	20.35	1.805	5.436	1.00	25.05
1572	C	PHE	A	686	22.387	-3.887	8.301	1.00	22.98
1573	CA	PHE	A	686	20.991	-3.391	7.89	1.00	23.92
1574	CB	PHE	A	686	20.211	-4.516	7.207	1.00	20.05
1575	CD1	PHE	A	686	19.237	-5.712	9.194	1.00	21.55
1576	CD2	PHE	A	686	20.775	-6.901	7.781	1.00	21.4
1577	CE1	PHE	A	686	19.131	-6.816	10.021	1.00	21.43
1578	CE2	PHE	A	686	20.673	-8.017	8.607	1.00	22.94
1579	CG	PHE	A	686	20.061	-5.737	8.066	1.00	22.24
1580	CZ	PHE	A	686	19.85	-7.971	9.728	1.00	23.48
1581	N	PHE	A	686	21.095	-2.211	7.033	1.00	23.24
1582	O	PHE	A	686	22.577	-4.409	9.414	1.00	23.52
1583	C	GLY	A	687	25.236	-3.254	8.865	1.00	21.88
1584	CA	GLY	A	687	24.721	-4.107	7.714	1.00	23.62
1585	N	GLY	A	687	23.352	-3.73	7.4	1.00	23.8

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1586	O	GLY	A	687	25.895	-3.762	9.775	1.00	23.55
1587	C	VAL	A	688	24.606	-1.404	11.19	1.00	22.9
1588	CA	VAL	A	688	25.339	-1.014	9.883	1.00	22.86
1589	CB	VAL	A	688	25.033	0.478	9.488	1.00	21.54
1590	CG1	VAL	A	688	25.553	1.447	10.54	1.00	21.4
1591	CG2	VAL	A	688	25.683	0.823	8.159	1.00	23.44
1592	N	VAL	A	688	24.937	-1.953	8.823	1.00	21.08
1593	O	VAL	A	688	25.203	-1.467	12.269	1.00	22.64
1594	C	LEU	A	689	23.171	-3.39	12.877	1.00	26.01
1595	CA	LEU	A	689	22.546	-2.121	12.264	1.00	25.16
1596	CB	LEU	A	689	21.073	-2.362	11.884	1.00	25.38
1597	CD1	LEU	A	689	18.654	-2.133	12.442	1.00	28.73
1598	CD2	LEU	A	689	19.985	-3.903	13.577	1.00	27.44
1599	CG	LEU	A	689	20.02	-2.502	13.001	1.00	29.51
1600	N	LEU	A	689	23.318	-1.709	11.089	1.00	22.99
1601	O	LEU	A	689	23.256	-3.511	14.102	1.00	26.52
1602	C	LEU	A	690	25.432	-5.172	13.357	1.00	25.2
1603	CA	LEU	A	690	24.23	-5.557	12.524	1.00	24.71
1604	CB	LEU	A	690	24.696	-6.45	11.379	1.00	26.58
1605	CD1	LEU	A	690	24.477	-7.957	9.432	1.00	26.44
1606	CD2	LEU	A	690	23.06	-8.389	11.475	1.00	24.02
1607	CG	LEU	A	690	23.711	-7.316	10.588	1.00	26.56
1608	N	LEU	A	690	23.596	-4.334	12.032	1.00	25.78
1609	O	LEU	A	690	25.641	-5.702	14.446	1.00	24.83
1610	C	TRP	A	691	27.02	-3.155	14.884	1.00	25.7
1611	CA	TRP	A	691	27.406	-3.734	13.513	1.00	25.21
1612	CB	TRP	A	691	28.072	-2.665	12.641	1.00	24.91
1613	CD1	TRP	A	691	30.64	-2.716	12.84	1.00	27.46
1614	CD2	TRP	A	691	29.636	-1.115	14.058	1.00	25.87
1615	CE2	TRP	A	691	31.038	-1.016	14.247	1.00	26.86
1616	CE3	TRP	A	691	28.798	-0.207	14.725	1.00	25.51
1617	CG	TRP	A	691	29.401	-2.2	13.157	1.00	27.51
1618	CH2	TRP	A	691	30.774	0.826	15.711	1.00	29.49
1619	CZ2	TRP	A	691	31.618	-0.047	15.072	1.00	26.62
1620	CZ3	TRP	A	691	29.375	0.753	15.546	1.00	27.28
1621	N	TRP	A	691	26.215	-4.236	12.833	1.00	26.85
1622	NE1	TRP	A	691	31.622	-2.006	13.494	1.00	28.59
1623	O	TRP	A	691	27.677	-3.431	15.893	1.00	24.24
1624	C	GLU	A	692	25.089	-2.853	17.196	1.00	26.74

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1625	CA	GLU	A	692	25.436	-1.787	16.166	1.00	25.95
1626	CB	GLU	A	692	24.179	-0.967	15.923	1.00	27.65
1627	CD	GLU	A	692	23.048	1.002	14.973	1.00	25.49
1628	CG	GLU	A	692	24.34	0.245	15.053	1.00	23.66
1629	N	GLU	A	692	25.926	-2.39	14.921	1.00	26.45
1630	O	GLU	A	692	25.331	2.67	18.385	1.00	29.64
1631	OE1	GLU	A	692	22.795	1.843	15.863	1.00	25.04
1632	OE2	GLU	A	692	22.262	0.731	14.047	1.00	22.01
1633	C	ILE	A	693	25.34	-5.692	18.249	1.00	28.02
1634	CA	ILE	A	693	24.112	-5.046	17.623	1.00	26.27
1635	CB	ILE	A	693	23.273	-6.141	16.868	1.00	25.63
1636	CD1	ILE	A	693	20.992	-6.49	15.649	1.00	22.33
1637	CG1	ILE	A	693	21.879	-5.577	16.517	1.00	25.07
1638	CG2	ILE	A	693	23.162	-7.439	17.713	1.00	21.79
1639	N	ILE	A	693	24.492	-3.95	16.739	1.00	26.22
1640	O	ILE	A	693	25.405	-5.878	19.461	1.00	28.08
1641	C	PHE	A	694	28.512	-5.776	18.682	1.00	31.7
1642	CA	PHE	A	694	27.523	-6.671	17.934	1.00	30.64
1643	CB	PHE	A	694	28.138	-7.559	16.848	1.00	27.9
1644	CD1	PHE	A	694	26.814	-9.659	17.246	1.00	32.04
1645	CD2	PHE	A	694	26.557	-8.537	15.148	1.00	33.22
1646	CE1	PHE	A	694	25.812	-10.563	16.901	1.00	31.91
1647	CE2	PHE	A	694	25.554	-9.436	14.794	1.00	33.38
1648	CG	PHE	A	694	27.191	-8.631	16.382	1.00	30.33
1649	CZ	PHE	A	694	25.179	-10.451	15.679	1.00	32.17
1650	N	PHE	A	694	26.331	-6.011	17.426	1.00	30.65
1651	O	PHE	A	694	29.481	-6.25	19.265	1.00	34.81
1652	C	THR	A	695	28.236	-3.117	20.652	1.00	30.5
1653	CA	THR	A	695	29.081	-3.56	19.452	1.00	30.28
1654	CB	THR	A	695	29.516	-2.341	18.638	1.00	28.44
1655	CG2	THR	A	695	30.44	-2.768	17.504	1.00	23.6
1656	N	THR	A	695	28.254	-4.475	18.685	1.00	31.37
1657	O	THR	A	695	28.636	-2.239	21.422	1.00	31.57
1658	OG1	THR	A	695	28.366	-1.673	18.109	1.00	30.24
1659	C	LEU	A	696	25.723	-2.017	21.969	1.00	28.27
1660	CA	LEU	A	696	26.121	-3.477	21.879	1.00	30.07
1661	CB	LEU	A	696	26.651	-3.965	23.231	1.00	33.28
1662	CD1	LEU	A	696	27.464	-5.777	24.723	1.00	34.16
1663	CD2	LEU	A	696	25.623	-6.217	23.104	1.00	36.84

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1664	CG	LEU	A	696	26.913	-5.464	23.346	1.00	33.11
1665	N	LEU	A	696	27.074	-3.754	20.801	1.00	28.35
1666	O	LEU	A	696	25.792	-1.411	23.024	1.00	28.9
1667	C	GLY	A	697	25.992	0.85	20.494	1.00	28.35
1668	CA	GLY	A	697	24.855	-0.078	20.85	1.00	28.73
1669	N	GLY	A	697	25.261	-1.467	20.858	1.00	28.67
1670	O	GLY	A	697	25.947	2.033	20.815	1.00	29.87
1671	C	GLY	A	698	27.762	2.212	18.391	1.00	32.66
1672	CA	GLY	A	698	28.126	1.138	19.397	1.00	31.19
1673	N	GLY	A	698	26.988	0.326	19.789	1.00	29.76
1674	O	GLY	A	698	26.825	2.055	17.615	1.00	33.47
1675	C	SER	A	699	29.222	4.316	16.282	1.00	32.24
1676	CA	SER	A	699	28.298	4.429	17.507	1.00	32.04
1677	CB	SER	A	699	28.562	5.734	18.28	1.00	34.6
1678	N	SER	A	699	28.513	3.303	18.405	1.00	30.94
1679	O	SER	A	699	30.446	4.361	16.403	1.00	32.03
1680	OG	SER	A	699	28.516	6.894	17.464	1.00	39.8
1681	C	PRO	A	700	30.254	5.299	13.627	1.00	28.74
1682	CA	PRO	A	700	29.453	4.021	13.862	1.00	31.94
1683	CB	PRO	A	700	28.39	3.85	12.758	1.00	32.24
1684	CD	PRO	A	700	27.206	4.121	14.762	1.00	34.12
1685	CG	PRO	A	700	27.19	3.331	13.486	1.00	33.2
1686	N	PRO	A	700	28.642	4.14	15.084	1.00	33
1687	O	PRO	A	700	29.751	6.381	13.888	1.00	28.29
1688	C	TYR	A	701	32.318	7.437	13.956	1.00	30.95
1689	CA	TYR	A	701	32.356	6.328	12.888	1.00	29.99
1690	CB	TYR	A	701	31.98	6.949	11.533	1.00	30.24
1691	CD1	TYR	A	701	33.191	5.453	9.894	1.00	37.01
1692	CD2	TYR	A	701	30.818	5.693	9.683	1.00	39.15
1693	CE1	TYR	A	701	33.211	4.61	8.784	1.00	42.54
1694	CE2	TYR	A	701	30.824	4.857	8.578	1.00	40.83
1695	CG	TYR	A	701	31.996	6.008	10.356	1.00	36.34
1696	CZ	TYR	A	701	32.018	4.32	8.128	1.00	44.67
1697	N	TYR	A	701	31.499	5.171	13.176	1.00	28.56
1698	O	TYR	A	701	31.973	8.582	13.665	1.00	31.66
1699	OH	TYR	A	701	32.007	3.52	6.999	1.00	52.98
1700	C	PRO	A	702	33.633	9.273	15.872	1.00	34.23
1701	CA	PRO	A	702	32.64	8.173	16.225	1.00	33.14
1702	CB	PRO	A	702	33.117	7.455	17.486	1.00	31.54

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1703	CD	PRO	A	702	33.211	5.865	15.755	1.00	37.25
1704	CG	PRO	A	702	32.873	6.022	17.217	1.00	40.43
1705	N	PRO	A	702	32.674	7.117	15.203	1.00	34.73
1706	O	PRO	A	702	34.756	8.983	15.442	1.00	33.47
1707	C	GLY	A	703	34.232	12.012	14.296	1.00	34.78
1708	CA	GLY	A	703	34.062	11.674	15.764	1.00	34.64
1709	N	GLY	A	703	33.21	10.525	16.042	1.00	36.58
1710	O	GLY	A	703	34.981	12.927	13.953	1.00	35.05
1711	C	VAL	A	704	32.5	12.42	11.501	1.00	32.98
1712	CA	VAL	A	704	33.629	11.515	11.987	1.00	32.62
1713	CB	VAL	A	704	33.589	10.18	11.199	1.00	31.21
1714	CG1	VAL	A	704	33.599	10.448	9.687	1.00	30.33
1715	CG2	VAL	A	704	34.765	9.286	11.605	1.00	28.15
1716	N	VAL	A	704	33.537	11.285	13.424	1.00	35.18
1717	O	VAL	A	704	31.325	12.085	11.631	1.00	33.71
1718	C	PRO	A	705	31.386	14.158	9.051	1.00	33.88
1719	CA	PRO	A	705	31.812	14.516	10.47	1.00	33.57
1720	CB	PRO	A	705	32.526	15.864	10.509	1.00	33.48
1721	CD	PRO	A	705	34.173	14.228	10.929	1.00	33.02
1722	CG	PRO	A	705	33.92	15.501	10.145	1.00	36.27
1723	N	PRO	A	705	32.84	13.597	10.962	1.00	32.36
1724	O	PRO	A	705	32.113	13.453	8.343	1.00	32.66
1725	C	VAL	A	706	30.711	14.468	6.157	1.00	31.8
1726	CA	VAL	A	706	29.676	14.461	7.291	1.00	33.71
1727	CB	VAL	A	706	28.579	15.507	6.971	1.00	36.55
1728	CG1	VAL	A	706	28.021	15.283	5.585	1.00	40.48
1729	CG2	VAL	A	706	27.457	15.423	7.99	1.00	38.28
1730	N	VAL	A	706	30.234	14.689	8.632	1.00	33.36
1731	O	VAL	A	706	30.849	13.491	5.422	1.00	32.21
1732	C	GLU	A	707	33.501	14.598	4.984	1.00	28.17
1733	CA	GLU	A	707	32.458	15.708	4.998	1.00	29.22
1734	CB	GLU	A	707	33.165	17.061	5.125	1.00	29.76
1735	N	GLU	A	707	31.437	15.57	6.027	1.00	30.95
1736	O	GLU	A	707	33.936	14.178	3.912	1.00	30.1
1737	C	GLU	A	708	34.33	11.74	5.881	1.00	28.89
1738	CA	GLU	A	708	34.937	13.089	6.238	1.00	28.94
1739	CB	GLU	A	708	35.565	13.016	7.634	1.00	31.31
1740	CD	GLU	A	708	37.415	14.736	7.22	1.00	49.17
1741	CG	GLU	A	708	36.256	14.293	8.097	1.00	40.8

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1742	N	GLU	A	708	33.928	14.143	6.16	1.00	28.61
1743	O	GLU	A	708	34.987	10.882	5.271	1.00	27.01
1744	OE1	GLU	A	708	38.049	13.889	6.546	1.00	52.8
1745	OE2	GLU	A	708	37.708	15.955	7.229	1.00	57.69
1746	C	LEU	A	709	32.278	10.122	4.448	1.00	28.41
1747	CA	LEU	A	709	32.367	10.318	5.961	1.00	29.05
1748	CB	LEU	A	709	30.965	10.325	6.58	1.00	28.83
1749	CD1	LEU	A	709	30.682	7.826	6.629	1.00	28.99
1750	CD2	LEU	A	709	28.679	9.335	6.575	1.00	29.38
1751	CG	LEU	A	709	30.107	9.143	6.118	1.00	30.91
1752	N	LEU	A	709	33.07	11.557	6.26	1.00	28.74
1753	O	LEU	A	709	32.436	9.003	3.952	1.00	29.22
1754	C	PHE	A	710	33.186	10.643	1.672	1.00	30.82
1755	CA	PHE	A	710	31.898	11.184	2.278	1.00	28.93
1756	CB	PHE	A	710	31.644	12.592	1.744	1.00	31.97
1757	CD1	PHE	A	710	29.274	12.272	2.517	1.00	42.62
1758	CD2	PHE	A	710	29.957	14.438	1.78	1.00	43.95
1759	CE1	PHE	A	710	27.991	12.752	2.776	1.00	46.1
1760	CE2	PHE	A	710	28.675	14.928	2.036	1.00	46.58
1761	CG	PHE	A	710	30.266	13.108	2.017	1.00	37.93
1762	CZ	PHE	A	710	27.691	14.079	2.537	1.00	44.57
1763	N	PHE	A	710	31.999	11.21	3.731	1.00	27.14
1764	O	PHE	A	710	33.162	9.79	0.782	1.00	29.22
1765	C	LYS	A	711	35.898	9.252	2.058	1.00	32.23
1766	CA	LYS	A	711	35.642	10.741	1.762	1.00	33.07
1767	CB	LYS	A	711	36.665	11.637	2.467	1.00	37.52
1768	CD	LYS	A	711	38.979	12.479	2.721	1.00	47.25
1769	CE	LYS	A	711	40.381	12.453	2.145	1.00	52.3
1770	CG	LYS	A	711	38.1	11.431	2.067	1.00	42.84
1771	N	LYS	A	711	34.304	11.138	2.193	1.00	31.29
1772	NZ	LYS	A	711	41.096	11.202	2.509	1.00	59.04
1773	O	LYS	A	711	36.41	8.522	1.204	1.00	30.89
1774	C	LEU	A	712	34.916	6.529	2.644	1.00	29.4
1775	CA	LEU	A	712	35.694	7.392	3.628	1.00	29.67
1776	CB	LEU	A	712	35.208	7.116	5.065	1.00	28.46
1777	CD1	LEU	A	712	35.406	7.318	7.566	1.00	26.91
1778	CD2	LEU	A	712	37.449	7.115	6.181	1.00	30.61
1779	CG	LEU	A	712	36.034	7.67	6.238	1.00	30.38
1780	N	LEU	A	712	35.527	8.8	3.258	1.00	31.38

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1781	O	LEU	A	712	35.441	5.545	2.126	1.00	31.08
1782	C	LEU	A	713	33.422	6.149	0.028	1.00	32.56
1783	CA	LEU	A	713	32.837	6.154	1.438	1.00	32.21
1784	CB	LEU	A	713	31.4	6.69	1.431	1.00	35.05
1785	CD1	LEU	A	713	29.302	7.07	2.763	1.00	41.06
1786	CD2	LEU	A	713	30.381	4.819	2.736	1.00	40.11
1787	CG	LEU	A	713	30.611	6.317	2.694	1.00	37.43
1788	N	LEU	A	713	33.669	6.905	2.376	1.00	30.38
1789	O	LEU	A	713	33.521	5.1	-0.609	1.00	32.11
1790	C	LYS	A	714	35.65	6.496	-1.893	1.00	34.98
1791	CA	LYS	A	714	34.414	7.389	-1.788	1.00	32.38
1792	CB	LYS	A	714	34.784	8.829	-2.129	1.00	32.84
1793	CD	LYS	A	714	32.71	9.23	-3.44	1.00	36.94
1794	CE	LYS	A	714	31.611	10.239	-3.736	1.00	40.9
1795	CG	LYS	A	714	33.59	9.725	-2.319	1.00	34.01
1796	N	LYS	A	714	33.834	7.313	-0.456	1.00	32.26
1797	NZ	LYS	A	714	30.717	9.816	-4.852	1.00	45.99
1798	O	LYS	A	714	35.932	5.922	-2.948	1.00	36.68
1799	C	GLU	A	715	37.307	4.061	-0.492	1.00	33.78
1800	CA	GLU	A	715	37.562	5.535	-0.765	1.00	35.28
1801	CB	GLU	A	715	38.562	6.14	0.216	1.00	37.64
1802	CD	GLU	A	715	39.718	8.336	0.83	1.00	50.74
1803	CG	GLU	A	715	38.966	7.54	-0.219	1.00	44.2
1804	N	GLU	A	715	36.358	6.342	-0.782	1.00	34.17
1805	O	GLU	A	715	38.242	3.269	-0.432	1.00	33.99
1806	OE1	GLU	A	715	39.952	7.828	1.951	1.00	50.09
1807	OE2	GLU	A	715	40.074	9.494	0.516	1.00	55.74
1808	C	GLY	A	716	35.968	1.795	1.262	1.00	28.5
1809	CA	GLY	A	716	35.679	2.313	-0.128	1.00	27.11
1810	N	GLY	A	716	36.035	3.695	-0.368	1.00	31.33
1811	O	GLY	A	716	36.103	0.593	1.453	1.00	27.84
1812	C	HIS	A	717	35.181	1.44	4.193	1.00	29.06
1813	CA	HIS	A	717	36.325	2.276	3.616	1.00	29.46
1814	CB	HIS	A	717	36.513	3.516	4.486	1.00	30.63
1815	CD2	HIS	A	717	37.967	3.092	6.6	1.00	32.86
1816	CE1	HIS	A	717	36.341	2.862	8.057	1.00	31.64
1817	CG	HIS	A	717	36.796	3.217	5.929	1.00	33.1
1818	N	HIS	A	717	36.055	2.686	2.242	1.00	29.11
1819	ND1	HIS	A	717	35.799	3.066	6.87	1.00	34.14

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1820	NE2	HIS	A	717	37.656	2.877	7.92	1.00	32.24
1821	O	HIS	A	717	34.019	1.704	3.909	1.00	30.87
1822	C	ARG	A	718	35.016	-0.515	7.151	1.00	30.57
1823	CA	ARG	A	718	34.56	-0.417	5.689	1.00	28.19
1824	CB	ARG	A	718	34.54	-1.811	5.062	1.00	29.38
1825	CD	ARG	A	718	32.603	-1.39	3.484	1.00	28.19
1826	CG	ARG	A	718	34.062	-1.859	3.613	1.00	28.65
1827	CZ	ARG	A	718	32.18	-0.472	1.211	1.00	25.18
1828	N	ARG	A	718	35.525	0.448	5.009	1.00	28.68
1829	NE	ARG	A	718	32.092	-1.456	2.105	1.00	25.18
1830	NH1	ARG	A	718	32.776	0.676	1.529	1.00	23.04
1831	NH2	ARG	A	718	31.611	-0.612	0.016	1.00	21.48
1832	O	ARG	A	718	36.213	-0.627	7.425	1.00	30.69
1833	C	MET	A	719	35.021	-1.791	9.864	1.00	30.44
1834	CA	MET	A	719	34.369	-0.472	9.514	1.00	31.8
1835	CB	MET	A	719	33.089	-0.297	10.336	1.00	34.76
1836	CE	MET	A	719	29.767	0.369	10.529	1.00	37.35
1837	CG	MET	A	719	32.418	1.058	10.185	1.00	37.05
1838	N	MET	A	719	34.076	-0.41	8.085	1.00	30.83
1839	O	MET	A	719	34.825	-2.778	9.172	1.00	31.9
1840	SD	MET	A	719	31.018	1.3	11.309	1.00	38.82
1841	C	ASP	A	720	35.524	-3.977	12.088	1.00	31.32
1842	CA	ASP	A	720	36.478	-3.012	11.399	1.00	33.86
1843	CB	ASP	A	720	37.604	-2.644	12.371	1.00	37.66
1844	CG	ASP	A	720	38.619	-1.669	11.774	1.00	44.55
1845	N	ASP	A	720	35.778	-1.808	10.954	1.00	32.94
1846	O	ASP	A	720	34.46	-3.576	12.56	1.00	32.08
1847	OD1	ASP	A	720	38.404	-1.172	10.641	1.00	51.07
1848	OD2	ASP	A	720	39.636	-1.39	12.455	1.00	47.71
1849	C	LYS	A	721	35.012	-6.048	14.31	1.00	35.5
1850	CA	LYS	A	721	35.112	-6.263	12.819	1.00	32.32
1851	CB	LYS	A	721	35.7	-7.657	12.58	1.00	33.3
1852	CD	LYS	A	721	35.341	-10.136	12.808	1.00	35.96
1853	CE	LYS	A	721	36.145	-10.676	13.961	1.00	41.96
1854	CG	LYS	A	721	34.814	-8.77	13.121	1.00	35.16
1855	N	LYS	A	721	35.934	-5.237	12.19	1.00	32.79
1856	NZ	LYS	A	721	36.407	-12.133	13.8	1.00	46.47
1857	O	LYS	A	721	36.035	-5.909	14.98	1.00	37.63
1858	C	PRO	A	722	34.238	-7.03	17.015	1.00	39.45



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1859	CA	PRO	A	722	33.614	-5.83	16.301	1.00	38.03
1860	CB	PRO	A	722	32.092	-5.857	16.475	1.00	36.29
1861	CD	PRO	A	722	32.474	-6.142	14.184	1.00	34.22
1862	CG	PRO	A	722	31.566	-5.412	15.121	1.00	34.41
1863	N	PRO	A	722	33.779	-6.024	14.856	1.00	36.8
1864	O	PRO	A	722	34.244	-8.142	16.472	1.00	39.16
1865	C	SER	A	723	34.118	-8.747	19.335	1.00	46.7
1866	CA	SER	A	723	35.362	-7.968	18.9	1.00	45.06
1867	CB	SER	A	723	36.199	-7.531	20.104	1.00	46.33
1868	N	SER	A	723	34.807	-6.826	18.198	1.00	43
1869	O	SER	A	723	33.012	-8.202	19.377	1.00	45.89
1870	OG	SER	A	723	35.398	-7.106	21.19	1.00	52.74
1871	C	ASN	A	724	32.02	-10.811	18.916	1.00	51.19
1872	CA	ASN	A	724	33.121	-10.829	19.997	1.00	52.69
1873	CB	ASN	A	724	32.612	-10.316	21.35	1.00	57.78
1874	CG	ASN	A	724	33.745	-10.151	22.368	1.00	62.15
1875	N	ASN	A	724	34.266	-10.039	19.568	1.00	47.68
1876	ND2	ASN	A	724	33.9	-8.942	22.891	1.00	63.89
1877	O	ASN	A	724	30.83	-10.62	19.18	1.00	51.72
1878	OD1	ASN	A	724	34.501	-11.091	22.635	1.00	63.26
1879	C	CYS	A	725	32.308	-12.118	15.617	1.00	41.7
1880	CA	CYS	A	725	31.597	-11.104	16.505	1.00	45.03
1881	CB	CYS	A	725	31.478	-9.738	15.829	1.00	43.73
1882	N	CYS	A	725	32.46	-11.033	17.684	1.00	48.4
1883	O	CYS	A	725	33.552	-12.061	15.472	1.00	44.04
1884	SG	CYS	A	725	30.705	-9.806	14.186	1.00	41.63
1885	C	THR	A	726	32.653	-13.602	12.922	1.00	33.1
1886	CA	THR	A	726	32.243	-14.132	14.311	1.00	34.56
1887	CB	THR	A	726	31.386	-15.419	14.22	1.00	33.03
1888	CG2	THR	A	726	31.169	-16.007	15.619	1.00	28.7
1889	N	THR	A	726	31.577	-13.104	15.11	1.00	36.81
1890	O	THR	A	726	32.158	-12.553	12.47	1.00	32.37
1891	OG1	THR	A	726	30.126	-15.114	13.611	1.00	34.07
1892	C	ASN	A	727	32.826	-13.997	10.029	1.00	34.32
1893	CA	ASN	A	727	34.036	-13.845	10.945	1.00	35.66
1894	CB	ASN	A	727	35.177	-14.701	10.401	1.00	40.52
1895	CG	ASN	A	727	36.477	-14.463	11.131	1.00	46.9
1896	N	ASN	A	727	33.613	-14.267	12.28	1.00	32.48
1897	ND2	ASN	A	727	36.977	-15.497	11.79	1.00	50.04

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FGFR1 COORDINATE DATA FOR RESIDUES 651-761

1898	O	ASN	A	727	32.661	-13.225	9.096	1.00	32.89
1899	OD1	ASN	A	727	37.034	-13.361	11.1	1.00	50.26
1900	C	GLU	A	728	29.815	-14.045	9.574	1.00	30.91
1901	CA	GLU	A	728	30.771	-15.235	9.531	1.00	31.99
1902	CB	GLU	A	728	30.064	-16.499	10.012	1.00	33.57
1903	CD	GLU	A	728	28.201	-18.183	9.618	1.00	38.97
1904	CG	GLU	A	728	28.841	-16.871	9.186	1.00	35.4
1905	N	GLU	A	728	31.974	-14.984	10.321	1.00	32.47
1906	O	GLU	A	728	29.33	-13.59	8.532	1.00	30
1907	OE1	GLU	A	728	28.223	-18.485	10.83	1.00	40.96
1908	OE2	GLU	A	728	27.671	-18.908	8.746	1.00	38.9
1909	C	LEU	A	729	29.303	-11.123	10.398	1.00	30.35
1910	CA	LEU	A	729	28.661	-12.399	10.927	1.00	30.1
1911	CB	LEU	A	729	28.215	-12.256	12.381	1.00	30.26
1912	CD1	LEU	A	729	27.137	-13.505	14.288	1.00	34.09
1913	CD2	LEU	A	729	25.832	-13.024	12.168	1.00	30.63
1914	CG	LEU	A	729	27.206	-13.346	12.77	1.00	34.27
1915	N	LEU	A	729	29.549	-13.539	10.775	1.00	29.99
1916	O	LEU	A	729	28.597	-10.217	9.956	1.00	29.1
1917	C	TYR	A	730	31.253	-9.933	8.372	1.00	27.66
1918	CA	TYR	A	730	31.328	-9.874	9.906	1.00	29.38
1919	CB	TYR	A	730	32.79	-9.833	10.361	1.00	29.47
1920	CD1	TYR	A	730	33.046	-7.334	10.071	1.00	30.48
1921	CD2	TYR	A	730	34.724	-8.759	9.125	1.00	29.99
1922	CE1	TYR	A	730	33.715	-6.214	9.589	1.00	29.16
1923	CE2	TYR	A	730	35.411	-7.633	8.635	1.00	28.76
1924	CG	TYR	A	730	33.537	-8.623	9.846	1.00	29.99
1925	CZ	TYR	A	730	34.893	-6.366	8.871	1.00	28.64
1926	N	TYR	A	730	30.636	-11.046	10.435	1.00	28.91
1927	O	TYR	A	730	31.079	-8.913	7.709	1.00	27.88
1928	OH	TYR	A	730	35.529	-5.242	8.378	1.00	32.2
1929	C	MET	A	731	29.915	-10.858	5.918	1.00	27.66
1930	CA	MET	A	731	31.298	-11.315	6.372	1.00	28.79
1931	CB	MET	A	731	31.518	-12.781	5.998	1.00	34.95
1932	CB	MET	A	731	32.582	-14.595	2.674	1.00	57.97
1933	CG	MET	A	731	31.168	-13.097	4.554	1.00	45.65
1934	N	MET	A	731	31.389	-11.132	7.814	1.00	26.76
1935	O	MET	A	731	29.775	-10.223	4.883	1.00	30.84
1936	SD	MET	A	731	31.431	-14.825	4.081	1.00	59.68

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1937	C	MET	A	732	27.446	-9.254	6.324	1.00	25.73
1938	CA	MET	A	732	27.523	-10.789	6.392	1.00	27.16
1939	CB	MET	A	732	26.566	-11.329	7.46	1.00	26.04
1940	CE	MET	A	732	23.786	-13.209	7.779	1.00	23.33
1941	CG	MET	A	732	25.124	-10.857	7.29	1.00	25.98
1942	N	MET	A	732	28.894	-11.205	6.69	1.00	28.89
1943	O	MET	A	732	26.887	-8.699	5.383	1.00	25.56
1944	SD	MET	A	732	24.008	-11.566	8.478	1.00	26.41
1945	C	MET	A	733	28.72	-6.616	6.056	1.00	28.1
1946	CA	MET	A	733	28.058	-7.119	7.329	1.00	27.05
1947	CB	MET	A	733	28.9	-6.614	8.488	1.00	25.68
1948	CE	MET	A	733	28.876	-7.106	12.431	1.00	29.07
1949	CG	MET	A	733	28.215	-6.548	9.811	1.00	31.65
1950	N	MET	A	733	28.028	-8.577	7.311	1.00	26.49
1951	O	MET	A	733	28.193	-5.74	5.388	1.00	31.02
1952	SD	MET	A	733	29.428	-6.102	11.081	1.00	29.98
1953	C	ARG	A	734	29.864	-7.03	3.253	1.00	23.89
1954	CA	ARG	A	734	30.637	-6.77	4.541	1.00	26.86
1955	CB	ARG	A	734	32.015	-7.456	4.504	1.00	25.68
1956	CD	ARG	A	734	33.24	-5.644	5.782	1.00	30.21
1957	CG	ARG	A	734	32.925	-7.127	5.712	1.00	27.93
1958	CZ	ARG	A	734	35.254	-5.361	4.382	1.00	44.7
1959	N	ARG	A	734	29.887	-7.172	5.734	1.00	28.31
1960	NE	ARG	A	734	33.94	-5.234	4.571	1.00	40.68
1961	NH1	ARG	A	734	36.028	-5.868	5.336	1.00	42.27
1962	NH2	ARG	A	734	35.779	-5.076	3.195	1.00	47.72
1963	O	ARG	A	734	29.998	-6.281	2.298	1.00	24.45
1964	C	ASP	A	735	27.144	-7.397	1.932	1.00	22.63
1965	CA	ASP	A	735	28.265	-8.425	2.051	1.00	23.43
1966	CB	ASP	A	735	27.685	-9.833	2.155	1.00	24.97
1967	CG	ASP	A	735	28.744	-10.917	2.028	1.00	27.28
1968	N	ASP	A	735	29.081	-8.102	3.222	1.00	24.55
1969	O	ASP	A	735	26.793	-6.979	0.827	1.00	23.12
1970	OD1	ASP	A	735	29.869	-10.633	1.553	1.00	27.47
1971	OD2	ASP	A	735	28.449	-12.061	2.409	1.00	28.68
1972	C	CYS	A	736	26.138	-4.641	2.603	1.00	23.2
1973	CA	CYS	A	736	25.562	-5.958	3.105	1.00	23.25
1974	CB	CYS	A	736	25.005	-5.779	4.53	1.00	21.44
1975	N	CYS	A	736	26.608	-6.974	3.076	1.00	20.37

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1976	O	CYS	A	736	25.418	-3.805	2.05	1.00	21.77
1977	SG	CYS	A	736	23.939	-7.138	5.092	1.00	21.74
1978	C	TRP	A	737	28.798	-3.378	0.982	1.00	25.19
1979	CA	TRP	A	737	28.125	-3.254	2.347	1.00	23.88
1980	CB	TRP	A	737	29.154	-2.8	3.376	1.00	19.59
1981	CD1	TRP	A	737	27.342	-2.016	4.997	1.00	23.18
1982	CD2	TRP	A	737	29.249	-2.675	5.965	1.00	24.7
1983	CE2	TRP	A	737	28.354	-2.261	6.977	1.00	25.57
1984	CE3	TRP	A	737	30.522	-3.143	6.339	1.00	28.72
1985	CG	TRP	A	737	28.59	-2.509	4.714	1.00	21.52
1986	CH2	TRP	A	737	29.937	-2.749	8.681	1.00	29.37
1987	CZ2	TRP	A	737	28.687	-2.29	8.341	1.00	26.08
1988	CZ3	TRP	A	737	30.854	-3.175	7.698	1.00	30.27
1989	N	TRP	A	737	27.446	-4.468	2.786	1.00	24.39
1990	NE1	TRP	A	737	27.192	-1.866	6.352	1.00	21.06
1991	O	TRP	A	737	29.764	-2.671	0.711	1.00	25.29
1992	C	HIS	A	738	28.732	-3.089	-1.964	1.00	25.9
1993	CA	HIS	A	738	28.906	-4.406	-1.199	1.00	24.58
1994	CB	HIS	A	738	28.308	-5.584	-1.999	1.00	25.27
1995	CD2	HIS	A	738	29.77	-5.414	-4.147	1.00	25.26
1996	CE1	HIS	A	738	30.524	-7.474	-4.188	1.00	26.77
1997	CG	HIS	A	738	29.209	-6.073	-3.102	1.00	25.99
1998	N	HIS	A	738	28.309	-4.272	0.123	1.00	25.8
1999	ND1	HIS	A	738	29.697	-7.364	-3.161	1.00	26.96
2000	NE2	HIS	A	738	30.585	-6.304	-4.801	1.00	30.67
2001	O	HIS	A	738	27.669	-2.455	-1.918	1.00	22.25
2002	C	ALA	A	739	28.674	-1.512	-4.465	1.00	25.22
2003	CA	ALA	A	739	29.77	-1.416	-3.391	1.00	24.98
2004	CB	ALA	A	739	31.147	-1.16	-4.03	1.00	26.79
2005	N	ALA	A	739	29.806	-2.646	-2.613	1.00	24.17
2006	O	ALA	A	739	27.953	-0.544	-4.724	1.00	27.56
2007	C	VAL	A	740	26.213	-3.36	-5.44	1.00	24.75
2008	CA	VAL	A	740	27.532	-2.915	-6.095	1.00	26.03
2009	CB	VAL	A	740	27.995	-3.996	-7.093	1.00	29.6
2010	CG1	VAL	A	740	27.06	-4.034	-8.305	1.00	25.61
2011	CG2	VAL	A	740	29.439	-3.731	-7.51	1.00	30.76
2012	N	VAL	A	740	28.546	-2.686	-5.072	1.00	22.08
2013	O	VAL	A	740	26.135	-4.471	-4.888	1.00	23.57
2014	C	PRO	A	741	23.281	-4.182	-5.321	1.00	21.81

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2015	CA	PRO	A	741	23.849	-2.829	-4.927	1.00	24
2016	CB	PRO	A	741	22.963	-1.679	-5.409	1.00	23.05
2017	CD	PRO	A	741	25.125	-1.19	-6.169	1.00	22.1
2018	CG	PRO	A	741	23.918	-0.532	-5.506	1.00	21.99
2019	N	PRO	A	741	25.158	-2.515	-5.519	1.00	24.91
2020	O	PRO	A	741	22.735	-4.884	-4.476	1.00	20.99
2021	C	SER	A	742	23.628	-7.052	-6.478	1.00	24.12
2022	CA	SER	A	742	22.936	-5.844	-7.091	1.00	24.28
2023	CB	SER	A	742	23.095	-5.92	-8.613	1.00	27.53
2024	N	SER	A	742	23.445	-4.565	-6.587	1.00	23.36
2025	O	SER	A	742	23.129	-8.17	-6.556	1.00	24.61
2026	OG	SER	A	742	24.463	-6.026	-8.98	1.00	29.14
2027	C	GLN	A	743	25.313	-8.161	-3.854	1.00	23.27
2028	CA	GLN	A	743	25.553	-7.924	-5.334	1.00	23.59
2029	CB	GLN	A	743	27.044	-7.749	-5.639	1.00	23.89
2030	CD	GLN	A	743	26.804	-9.049	-7.796	1.00	24.26
2031	CG	GLN	A	743	27.354	-7.794	-7.135	1.00	22.56
2032	N	GLN	A	743	24.806	-6.834	-5.912	1.00	24.23
2033	NE2	GLN	A	743	25.748	-8.896	-8.603	1.00	22.61
2034	O	GLN	A	743	25.852	-9.114	-3.299	1.00	25.08
2035	OE1	GLN	A	743	27.307	-10.143	-7.567	1.00	21.87
2036	C	ARG	A	744	23.178	-8.531	-1.612	1.00	22.5
2037	CA	ARG	A	744	24.226	-7.442	-1.79	1.00	21.92
2038	CB	ARG	A	744	23.691	-6.124	-1.216	1.00	19.87
2039	CD	ARG	A	744	24.057	-3.651	-0.909	1.00	20.26
2040	CG	ARG	A	744	24.674	-4.981	-1.322	1.00	21
2041	CZ	ARG	A	744	24.579	-1.329	-1.603	1.00	24.5
2042	N	ARG	A	744	24.525	-7.298	-3.213	1.00	23.61
2043	NE	ARG	A	744	24.944	-2.576	-1.325	1.00	25.51
2044	NH1	ARG	A	744	23.3	-0.952	-1.501	1.00	21.85
2045	NH2	ARG	A	744	25.499	-0.476	-2.052	1.00	20.11
2046	O	ARG	A	744	22.471	-8.881	-2.577	1.00	23.44
2047	C	PRO	A	745	20.8	-9.521	-0.042	1.00	23.46
2048	CA	PRO	A	745	22.149	-10.215	-0.22	1.00	21.95
2049	CB	PRO	A	745	22.599	-10.873	1.084	1.00	20.69
2050	CD	PRO	A	745	24.086	-9.111	0.717	1.00	20.62
2051	CG	PRO	A	745	23.294	-9.754	1.816	1.00	20.27
2052	N	PRO	A	745	23.154	-9.178	-0.428	1.00	20.74
2053	O	PRO	A	745	20.743	-8.319	0.233	1.00	25.66

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2054	C	THR	A	746	18.006	-9.962	1.367	1.00	25.27
2055	CA	THR	A	746	18.398	-9.684	-0.075	1.00	22.53
2056	CB	THR	A	746	17.379	-10.368	-1.005	1.00	21.83
2057	CG2	THR	A	746	17.716	-10.084	-2.467	1.00	24.13
2058	N	THR	A	746	19.72	-10.25	-0.258	1.00	23.66
2059	O	THR	A	746	18.67	-10.755	2.053	1.00	24.34
2060	OG1	THR	A	746	17.401	-11.788	-0.787	1.00	22.26
2061	C	PHE	A	747	16.03	-11.047	3.308	1.00	23.04
2062	CA	PHE	A	747	16.492	-9.593	3.214	1.00	24.91
2063	CB	PHE	A	747	15.385	-8.623	3.657	1.00	23.83
2064	CD1	PHE	A	747	16.723	-7.16	5.212	1.00	20.59
2065	CD2	PHE	A	747	15.627	-6.128	3.341	1.00	20.48
2066	CE1	PHE	A	747	17.263	-5.925	5.58	1.00	21.28
2067	CE2	PHE	A	747	16.156	-4.897	3.697	1.00	19.62
2068	CG	PHE	A	747	15.906	-7.274	4.089	1.00	23.69
2069	CZ	PHE	A	747	16.981	-4.795	4.826	1.00	18.59
2070	N	PHE	A	747	16.943	-9.318	1.848	1.00	25.21
2071	O	PHE	A	747	16.195	-11.693	4.341	1.00	24.81
2072	C	LYS	A	748	16.256	-13.866	2.448	1.00	25.48
2073	CA	LYS	A	748	15.055	-12.964	2.17	1.00	23.4
2074	CB	LYS	A	748	14.456	-13.291	0.801	1.00	26.59
2075	CD	LYS	A	748	13.642	-14.999	-0.831	1.00	37.13
2076	CE	LYS	A	748	13.237	-16.444	-1.093	1.00	43.19
2077	CG	LYS	A	748	14.019	-14.747	0.624	1.00	29.81
2078	N	LYS	A	748	15.504	-11.578	2.207	1.00	22.66
2079	NZ	LYS	A	748	12.075	-16.859	-0.246	1.00	52.96
2080	O	LYS	A	748	16.173	-14.785	3.269	1.00	27.15
2081	C	GLN	A	749	19.104	-14.213	3.39	1.00	23.84
2082	CA	GLN	A	749	18.592	-14.378	1.961	1.00	26.63
2083	CB	GLN	A	749	19.703	-13.921	1.008	1.00	28.76
2084	CD	GLN	A	749	20.521	-13.39	-1.308	1.00	40.15
2085	CG	GLN	A	749	19.413	-14.022	-0.472	1.00	37.08
2086	N	GLN	A	749	17.573	-13.594	1.773	1.00	24.72
2087	NE2	GLN	A	749	21.743	-13.902	-1.163	1.00	46.9
2088	O	GLN	A	749	19.468	-15.188	4.044	1.00	25.22
2089	OE1	GLN	A	749	20.295	-12.429	-2.028	1.00	38.37
2090	C	LEU	A	750	18.844	-13.391	6.258	1.00	27.69
2091	CA	LEU	A	750	19.654	-12.663	5.197	1.00	24.23
2092	CB	LEU	A	750	19.636	-11.152	5.445	1.00	23.26

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2093	CD1	LEU	A	750	20.273	-8.83	4.717	1.00	21.91
2094	CD2	LEU	A	750	22.039	-10.558	5.28	1.00	24.74
2095	CG	LEU	A	750	20.662	-10.322	4.676	1.00	23.65
2096	N	LEU	A	750	19.166	-12.969	3.848	1.00	23.32
2097	O	LEU	A	750	19.402	-13.899	7.241	1.00	27.59
2098	C	VAL	A	751	17.047	-15.631	7.035	1.00	26.42
2099	CA	VAL	A	751	16.66	-14.164	6.974	1.00	25.59
2100	CB	VAL	A	751	15.17	-13.984	6.591	1.00	26.06
2101	CG1	VAL	A	751	14.285	-14.975	7.352	1.00	27.79
2102	CG2	VAL	A	751	14.729	-12.597	6.944	1.00	21.17
2103	N	VAL	A	751	17.533	-13.48	6.039	1.00	27.44
2104	O	VAL	A	751	17.191	-16.201	8.118	1.00	23.41
2105	C	GLU	A	752	18.988	-17.892	6.496	1.00	33.15
2106	CA	GLU	A	752	17.631	-17.645	5.818	1.00	33.19
2107	CB	GLU	A	752	17.661	-18.13	4.37	1.00	35.99
2108	CD	GLU	A	752	16.33	-18.622	2.264	1.00	47.91
2109	CG	GLU	A	752	16.292	-18.11	3.694	1.00	42.9
2110	N	GLU	A	752	17.246	-16.238	5.87	1.00	30.11
2111	O	GLU	A	752	19.142	-18.831	7.289	1.00	30.94
2112	OE1	GLU	A	752	17.227	-19.436	1.942	1.00	54.41
2113	OE2	GLU	A	752	15.46	-18.217	1.465	1.00	46.86
2114	C	ASP	A	753	21.228	-16.993	8.295	1.00	28.98
2115	CA	ASP	A	753	21.286	-17.172	6.779	1.00	30.8
2116	CB	ASP	A	753	22.263	-16.169	6.154	1.00	29.39
2117	CG	ASP	A	753	22.503	-16.426	4.675	1.00	33.34
2118	N	ASP	A	753	19.961	-17.04	6.191	1.00	31.34
2119	O	ASP	A	753	21.763	-17.814	9.043	1.00	29.21
2120	OD1	ASP	A	753	22.382	-17.582	4.236	1.00	35.4
2121	OD2	ASP	A	753	22.819	-15.467	3.942	1.00	38.34
2122	C	LEU	A	754	19.697	-16.8	10.918	1.00	31.83
2123	CA	LEU	A	754	20.429	-15.687	10.19	1.00	28.42
2124	CB	LEU	A	754	19.759	-14.343	10.447	1.00	23.48
2125	CD1	LEU	A	754	20.015	-11.885	10.086	1.00	19.28
2126	CD2	LEU	A	754	21.858	-13.226	11.228	1.00	21.18
2127	CG	LEU	A	754	20.746	-13.218	10.161	1.00	25.55
2128	N	LEU	A	754	20.542	-15.951	8.752	1.00	27.47
2129	O	LEU	A	754	20.054	-17.155	12.041	1.00	32.48
2130	C	ASP	A	755	18.888	-19.634	11.062	1.00	34.6
2131	CA	ASP	A	755	17.935	-18.469	10.828	1.00	33.9

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TABLE 10  
FGFR1 COORDINATE DATA FOR RESIDUES 651-761

2132	CB	ASP	A	755	16.815	-18.879	9.877	1.00	36.88
2133	CG	ASP	A	755	15.821	-19.797	10.53	1.00	43.04
2134	N	ASP	A	755	18.699	-17.376	10.254	1.00	32.67
2135	O	ASP	A	755	18.823	-20.315	12.095	1.00	35.96
2136	OD1	ASP	A	755	15.344	-19.466	11.634	1.00	45.74
2137	OD2	ASP	A	755	15.525	-20.858	9.953	1.00	50.7
2138	C	ARG	A	756	21.759	-20.61	11.337	1.00	35.21
2139	CA	ARG	A	756	20.791	-20.883	10.185	1.00	34.08
2140	CB	ARG	A	756	21.548	-20.953	8.861	1.00	34.96
2141	CD	ARG	A	756	23.206	-22.112	7.387	1.00	43.2
2142	CG	ARG	A	756	22.63	-22.022	8.792	1.00	40.86
2143	CZ	ARG	A	756	24.873	-20.29	7.326	1.00	50
2144	N	ARG	A	756	19.793	-19.831	10.11	1.00	32.47
2145	NE	ARG	A	756	23.728	-20.829	6.918	1.00	48.98
2146	NH1	ARG	A	756	25.63	-20.925	8.219	1.00	49.87
2147	NH2	ARG	A	756	25.261	-19.116	6.84	1.00	51.25
2148	O	ARG	A	756	21.942	-21.446	12.219	1.00	37.36
2149	C	ILE	A	757	22.706	-19.046	13.802	1.00	36.18
2150	CA	ILE	A	757	23.282	-19.029	12.389	1.00	35.36
2151	CB	ILE	A	757	23.915	-17.648	12.101	1.00	34.7
2152	CD1	ILE	A	757	24.895	-16.284	10.172	1.00	31.43
2153	CG1	ILE	A	757	24.56	-17.655	10.712	1.00	33.5
2154	CG2	ILE	A	757	24.964	-17.32	13.161	1.00	32.03
2155	N	ILE	A	757	22.324	-19.41	11.359	1.00	35.79
2156	O	ILE	A	757	23.349	-19.562	14.709	1.00	35.75
2157	C	VAL	A	758	20.897	-19.911	15.922	1.00	41.26
2158	CA	VAL	A	758	20.889	-18.505	15.332	1.00	38.47
2159	CB	VAL	A	758	19.434	-17.963	15.32	1.00	37.23
2160	CG1	VAL	A	758	18.8	-18.072	16.719	1.00	38.22
2161	CG2	VAL	A	758	19.414	-16.523	14.857	1.00	35.36
2162	N	VAL	A	758	21.494	-18.527	13.994	1.00	36.59
2163	O	VAL	A	758	21.429	-20.134	17.019	1.00	42.29
2164	C	ALA	A	759	21.682	-22.792	15.931	1.00	42.41
2165	CA	ALA	A	759	20.303	-22.246	15.557	1.00	40.75
2166	CB	ALA	A	759	19.705	-23.069	14.443	1.00	39.82
2167	N	ALA	A	759	20.361	-20.855	15.154	1.00	40.43
2168	O	ALA	A	759	21.802	-23.625	16.82	1.00	44.86
2169	C	LEU	A	760	24.813	-21.967	16.573	1.00	47.37
2170	CA	LEU	A	760	24.074	-22.787	15.512	1.00	46.6



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TABLE 10  
FGFR1 COORDINATE DATA FOR RESIDUES 651-761

2171	CB	LEU	A	760	24.881	-22.766	14.212	1.00	47.18
2172	CD1	LEU	A	760	24.877	-23.326	11.775	1.00	55.68
2173	CD2	LEU	A	760	24.444	-25.118	13.501	1.00	52.42
2174	CG	LEU	A	760	24.266	-23.646	13.128	1.00	52.28
2175	N	LEU	A	760	22.717	-22.328	15.247	1.00	43.11
2176	O	LEU	A	760	25.926	-22.317	16.972	1.00	46.75
2177	C	THR	A	761	24.684	-20.468	19.464	1.00	50.19
2178	CA	THR	A	761	24.849	-20.024	18.011	1.00	49.57
2179	CB	THR	A	761	24.431	-18.536	17.811	1.00	49.71
2180	CG2	THR	A	761	25.043	-17.652	18.877	1.00	48.97
2181	N	THR	A	761	24.204	-20.883	17.034	1.00	49
2182	O	THR	A	761	23.587	-20.801	19.915	1.00	48.96
2183	OG1	THR	A	761	24.915	-18.076	16.543	1.00	49.18

It will be understood that various details of the invention can be changed without departing from the scope of the invention. Furthermore, the foregoing description is for the purpose of illustration only, and not for the purpose of limitation-- the invention being defined by the claims.

CLAIMS

What is claimed is:

1. A composition comprising a cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide in monoclinic crystalline form.
2. The composition of claim 1, wherein the crystalline form has lattice constants of  $a = 66 \text{ \AA}$ ,  $b = 92 \text{ \AA}$ ,  $c = 70 \text{ \AA}$ ,  $\alpha = 90^\circ$ ,  $\beta = 108^\circ$ ,  $\gamma = 90^\circ$ .
3. The composition of claim 1 or 2, wherein the crystalline form has a space group of  $P2_1$ .
4. The composition of claim 1 or 2, wherein the cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide has the amino acid sequence shown in SEQ ID NO: 4.
5. The composition of claim 1 or 2, wherein the cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide is unphosphorylated.
6. The composition of claim 1 or 2, wherein the Tie2K receptor tyrosine kinase domain has a crystalline structure further characterized by the coordinates corresponding to Table 2.
7. The composition of claim 1 or 2, wherein the crystalline form contains two molecules in the asymmetric unit.

8. The composition of claim 1 or 2, wherein the crystalline form is such that the three-dimensional structure of the crystallized cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide can be determined to a resolution of about 2.2 Å or better.

9. The composition of claim 1, wherein the crystalline form has lattice constants of  $a = 79 \text{ Å}$ ,  $b = 92 \text{ Å}$ ,  $c = 109 \text{ Å}$ ,  $\alpha = 90^\circ$ ,  $\beta = 90^\circ$ ,  $\gamma = 90^\circ$ .

10. The composition of claim 1, wherein the crystalline form has lattice constants of  $a = 52 \text{ Å}$ ,  $b = 77 \text{ Å}$ ,  $c = 79 \text{ Å}$ ,  $\alpha = 90^\circ$ ,  $\beta = 90^\circ$ ,  $\gamma = 90^\circ$ .

11. The composition of claim 1, 9 or 10, wherein the crystalline form has a space group of  $P2_12_12_1$ .

12. The composition of claim 1, 9 or 10, wherein the cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide has the amino acid sequence shown in SEQ ID NO: 4.

13. The composition of claim 1 or 9, wherein the cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide is unphosphorylated.

14. The composition of claim 1 or 10, wherein the cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide is monophosphorylated.

15. The composition of claim 1 or 9, wherein the Tie2K receptor tyrosine kinase domain has a crystalline structure further characterized by the coordinates corresponding to Table 3.

16. The composition of claim 1 or 10, wherein the Tie2K receptor tyrosine kinase domain has a crystalline structure further characterized by the coordinates corresponding to Table 4.

17. The composition of claims 1 or 9, wherein the crystalline form contains two molecules in the asymmetric unit.

18. The composition of claims 1 or 10, wherein the crystalline form contains one molecule in the asymmetric unit.

19. The composition of claim 1 or 9, wherein the crystalline form is such that the three-dimensional structure of the crystallized cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide can be determined to a resolution of about 2.5 Å or better.

20. The composition of claim 1 or 10, wherein the crystalline form is such that the three-dimensional structure of the crystallized cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide can be determined to a resolution of about 2.2 Å or better.

21. A composition comprising cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide in orthorhombic crystalline form.

22. The composition of claim 21 wherein the crystalline form has lattice constants of  $a = 95 \text{ \AA}$ ,  $b = 114 \text{ \AA}$ ,  $c = 78 \text{ \AA}$ ,  $\alpha = 90^\circ$ ,  $\beta = 90^\circ$ ,  $\gamma = 90^\circ$ .

23. The composition of claim 21 or 22 wherein the cytoplasmic Tie2 receptor tyrosine kinase has the amino acid sequence shown in SEQ ID NO: 6.

24. The composition of claim 21 or 22, wherein the crystalline form has a space group of  $C222_1$ .

25. The composition of claim 21 or 22 wherein the Tie2 receptor tyrosine kinase domain polypeptide is unphosphorylated.

26. The composition of claim 21 or 22, wherein the Tie2K receptor tyrosine kinase domain has a crystalline structure further characterized by the coordinates corresponding to Table 5.

27. The composition of claim 22, wherein the crystalline form is such that the three-dimensional structure of the crystallized cytoplasmic Tie2

receptor tyrosine kinase domain polypeptide can be determined to a resolution of about 2.1 Å or better.

28. A method for determining the three-dimensional structure of a crystallized cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide to a resolution of about 2.2 Å or better comprising:

- (a) crystallizing the cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide; and
- (b) analyzing the cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide to determine the three-dimensional structure of the crystallized Tie2 receptor tyrosine kinase domain polypeptide.

29. The method of claim 28, wherein the analyzing is by X-ray diffraction.

30. The method of claim 28, wherein the crystallization is accomplished using the hanging drop vapor diffusion method, wherein the cytoplasmic Tie2 receptor tyrosine kinase domain is mixed with an equal volume of reservoir.

31. The method of claim 30, wherein the reservoir comprises 2.5% PEG 1200, 2.5% glycerol, 100 mM HEPES at pH 7.5 and 10 mM spermidine.

32. The method of claim 30, wherein the reservoir comprises 100 mM HEPES at pH 7.5, 100 mM KCl and 10% isopropanol.

33. The method of claim 30, wherein the reservoir comprises 100 mM HEPES at pH 7.5 and 1.5 M NaCl.

34. A crystallized cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide produced by the method of claim 30.

35. A method of designing a modulator of a cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide, the method comprising:

- (a) designing a potential modulator of the cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide that will form bonds with amino acids in a substrate binding site based upon a crystalline structure of the cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide;
- (b) synthesizing the modulator; and
- (c) determining whether the potential modulator modulates the activity of the cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide.

36. A method of designing a modulator of a cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide the method comprising:



- (a) obtaining a monoclinic or orthorhombic crystal of a cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide;
- (b) evaluating the three-dimensional structure of the crystallized cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide; and
- (c) synthesizing a potential modulator based on the three-dimensional crystal structure of the crystallized cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide.

37. The method of claim 36, further comprising contacting a cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide with the potential modulator; and assaying the cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide for binding of the potential modulator, for a change in activity of the cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide, or both.

38. The method of claim 36, wherein the crystals are such that the three-dimensional structure of the crystallized cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide can be determined to a resolution of about 2.2 Å or better.

39. A method of screening for a modulator of a cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide, the method comprising:

- (a) providing a library of test samples;

- (b) contacting a crystalline form of a cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide with each test sample;
- (c) detecting an interaction between a test sample and the crystalline form of cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide;
- (d) identifying a test sample that interacts with the cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide; and
- (e) isolating a test sample that interacts with the cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide.

40. The method of claim 39, wherein the test samples are bound to a substrate.

41. The method of claim 39, wherein the test samples are synthesized directly on a substrate.

42. A cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide having at least one mutation in the amino acid sequence of the polypeptide, wherein the mutation is selected from the group consisting of Y897F, Y1048F or S1119A.

43. An isolated and substantially pure nucleic acid sequence encoding a cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide of claim 42.

44. An isolated and substantially pure nucleic acid sequence encoding a cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide of claim 42, wherein the nucleic acid sequence comprises the sequence shown in SEQ ID NO: 5.

45. An isolated and substantially pure nucleic acid sequence encoding a cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide of claim 42, wherein the nucleic acid sequence comprises a sequence having at least 70% sequence identity with the nucleic acid sequence shown in SEQ ID NO: 5.

46. A nucleic acid sequence which hybridizes to and is at least 70% complementary to the nucleic acid sequence of claim 43.

47. The nucleic acid sequence of claim 46, wherein hybridization conditions comprise 6X SSC; 0.2% polyvinylpyrrolidone; 0.2% Ficoll; 0.2% bovine serum albumin; 0.1% sodium dodecyl sulfate; 100 :gram/ml salmon sperm DNA and 15% formamide at 68° C.

48. A recombinant vector comprising a nucleic acid sequence of claim 43.

49. The recombinant vector of claim 48, further comprising:

- (a) a sequence of genomic viral DNA showing affinity for host cells and possessing the ability to infect said host cells;
- (b) a segment of DNA having the nucleic acid sequence shown in SEQ ID NO: 5 operatively linked to the sequence of genomic viral DNA, wherein the operatively-linked nucleic acid sequence shown in SEQ ID NO: 5 is expressed in said host cell following infection of the cell; and
- (c) a selectable marker.

50. A substantially pure preparation of a cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide of claim 42, wherein the polypeptide has the amino acid sequence shown in SEQ ID NO: 6.

51. A substantially pure preparation of a cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide of claim 42, wherein the polypeptide has at least 70% sequence identity with the amino acid sequence shown in SEQ ID NO: 6.

52. The substantially pure preparation of a cytoplasmic Tie2 receptor tyrosine kinase domain polypeptide of claim 50 or claim 51, wherein the polypeptide has autophosphorylation activity.

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FIG. 1

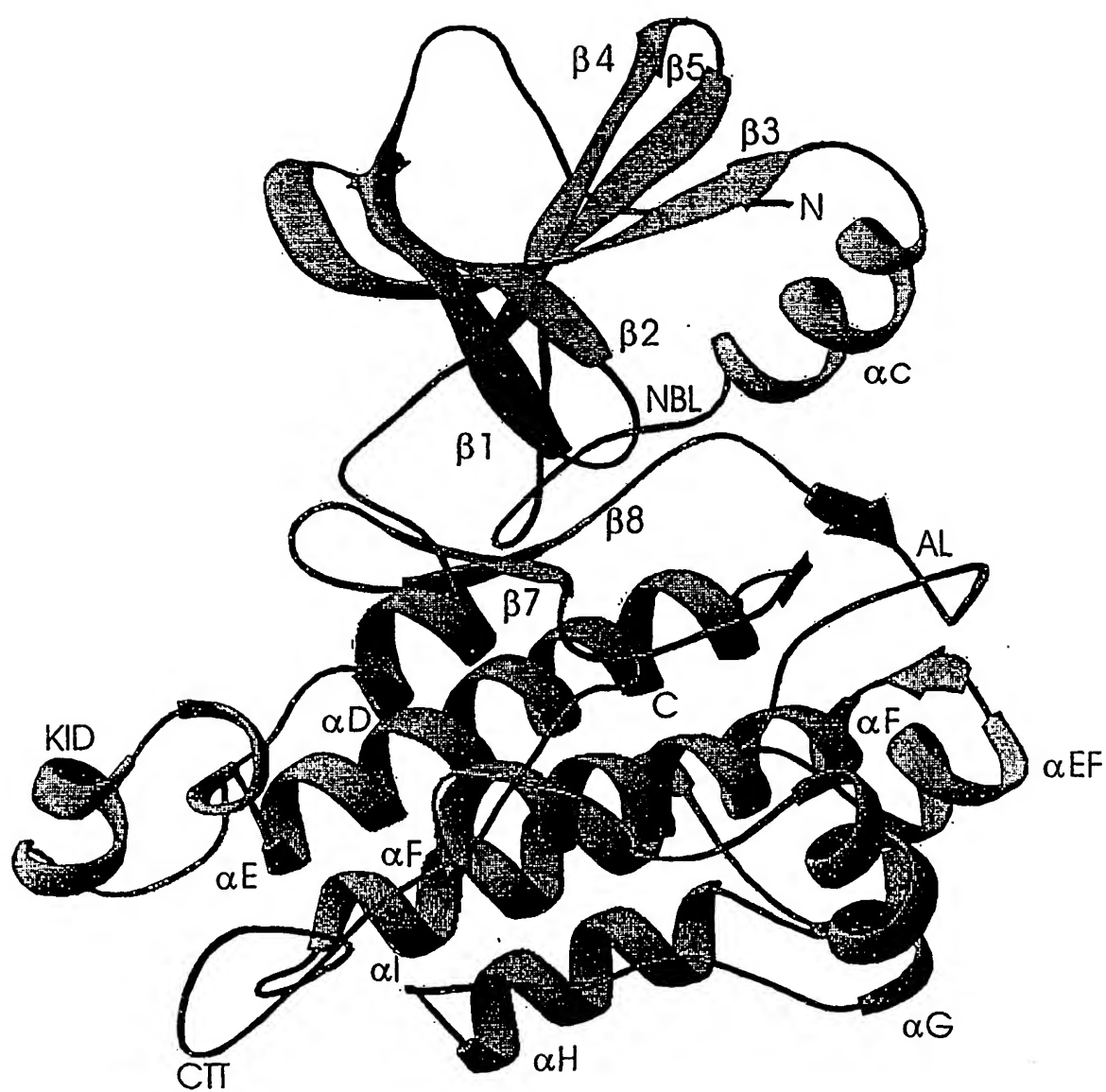
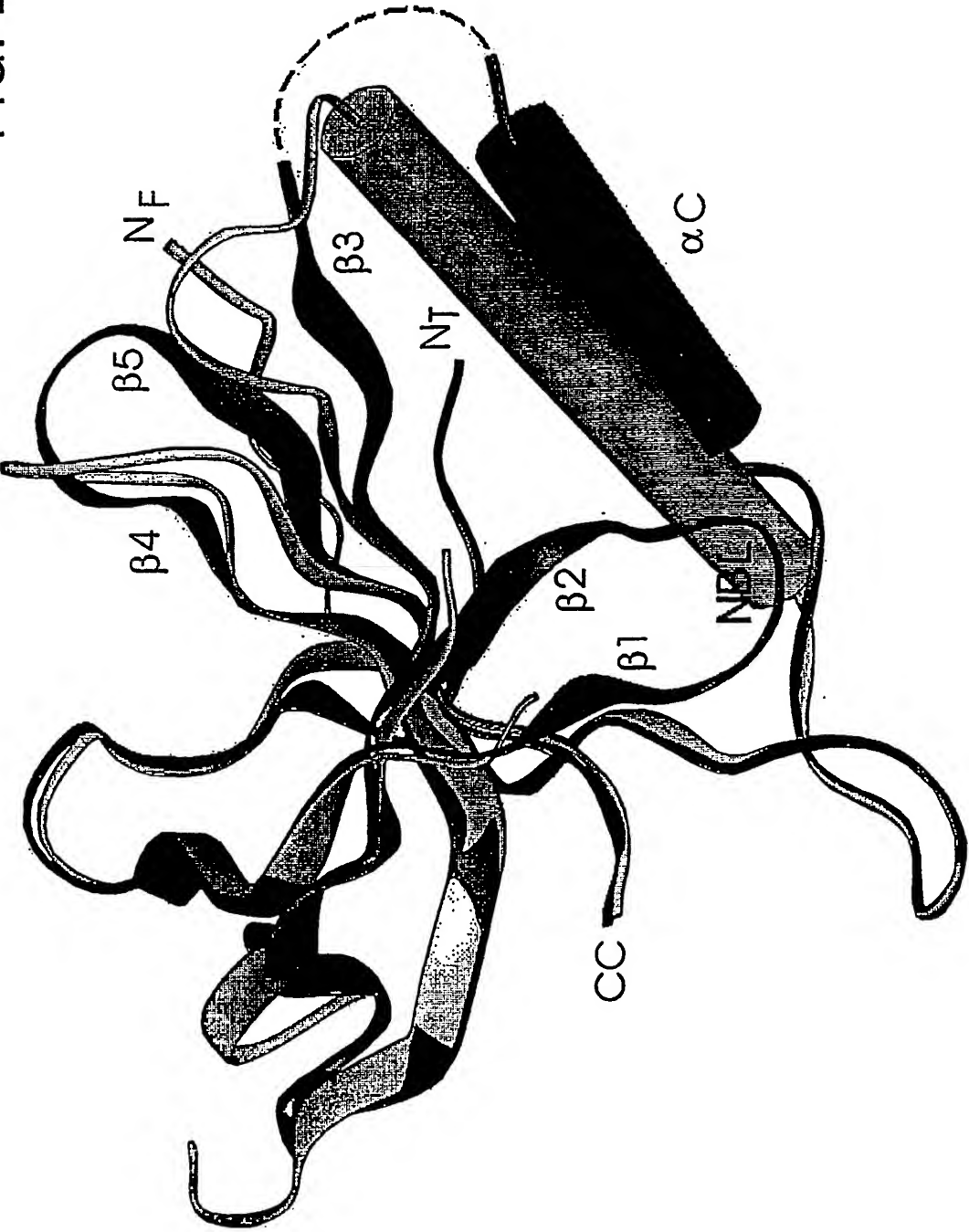
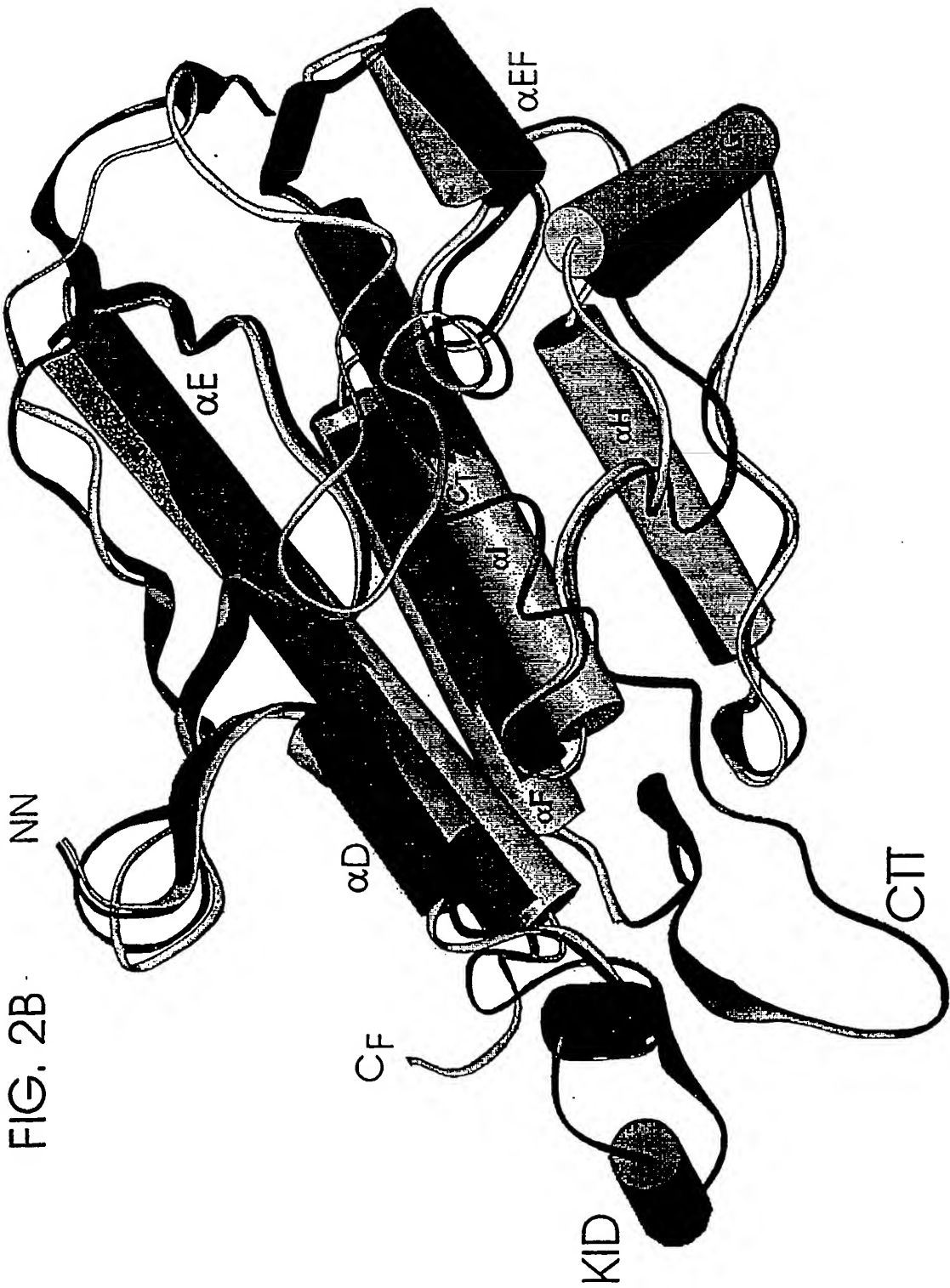


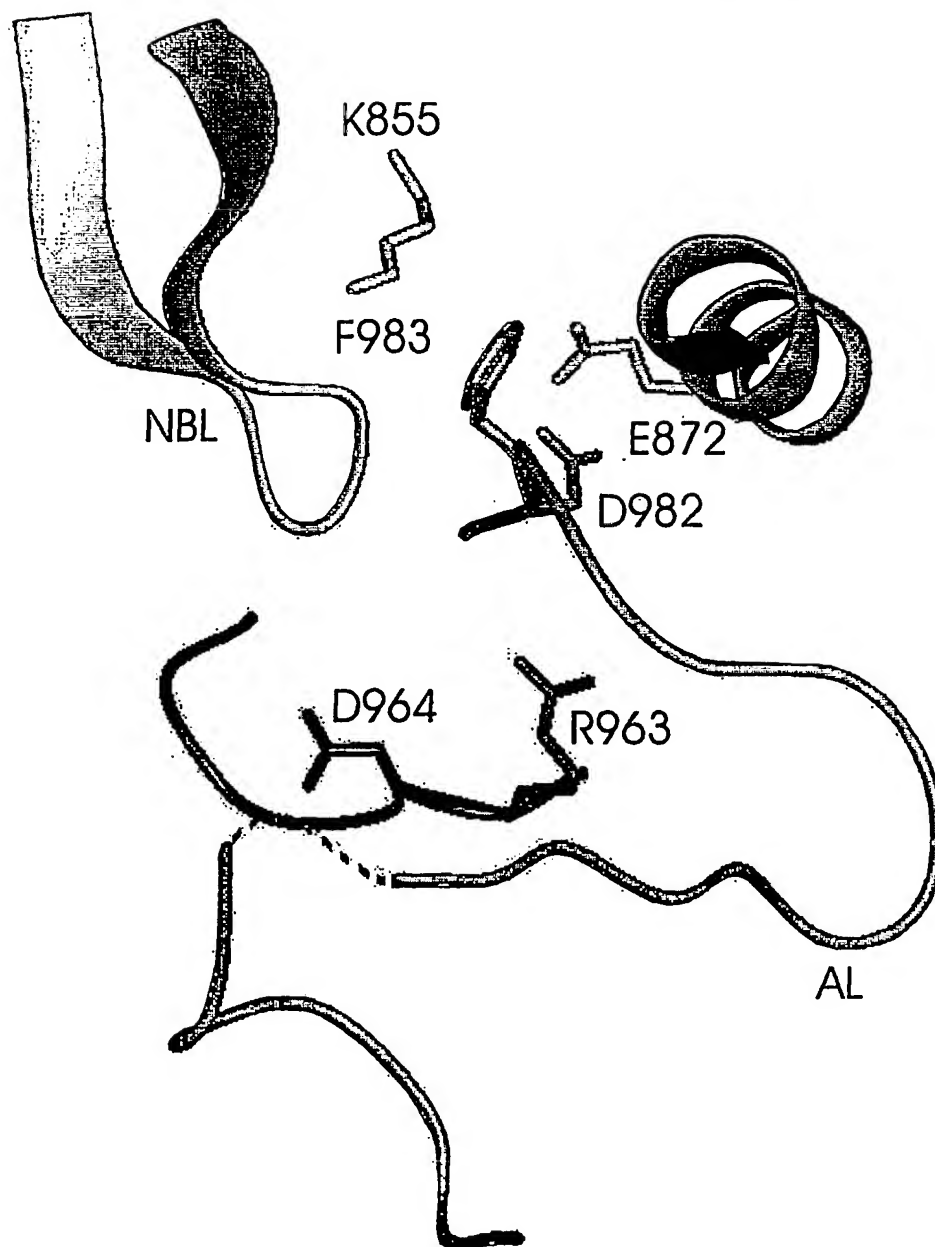
FIG. 2A





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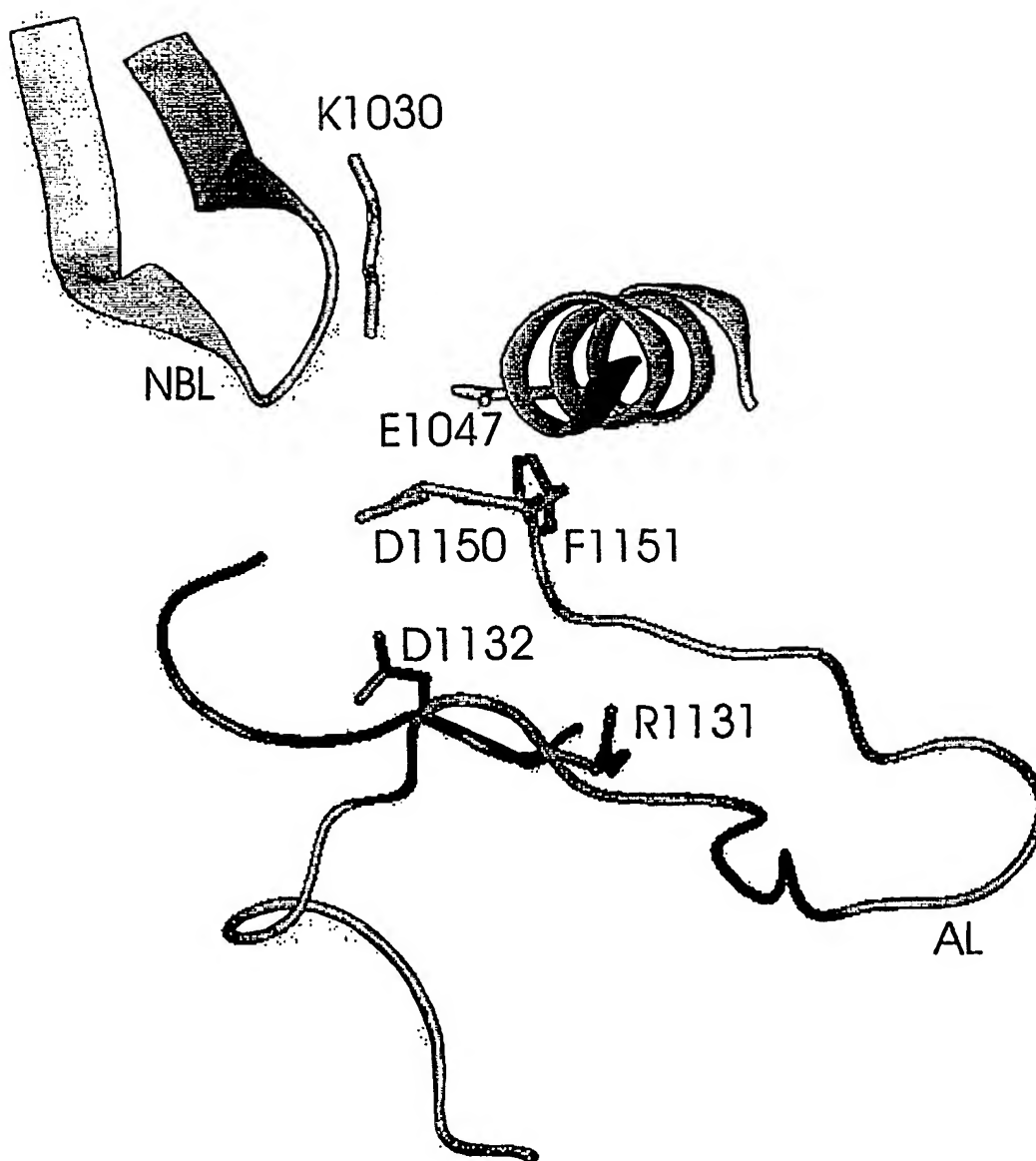
FIG. 3A





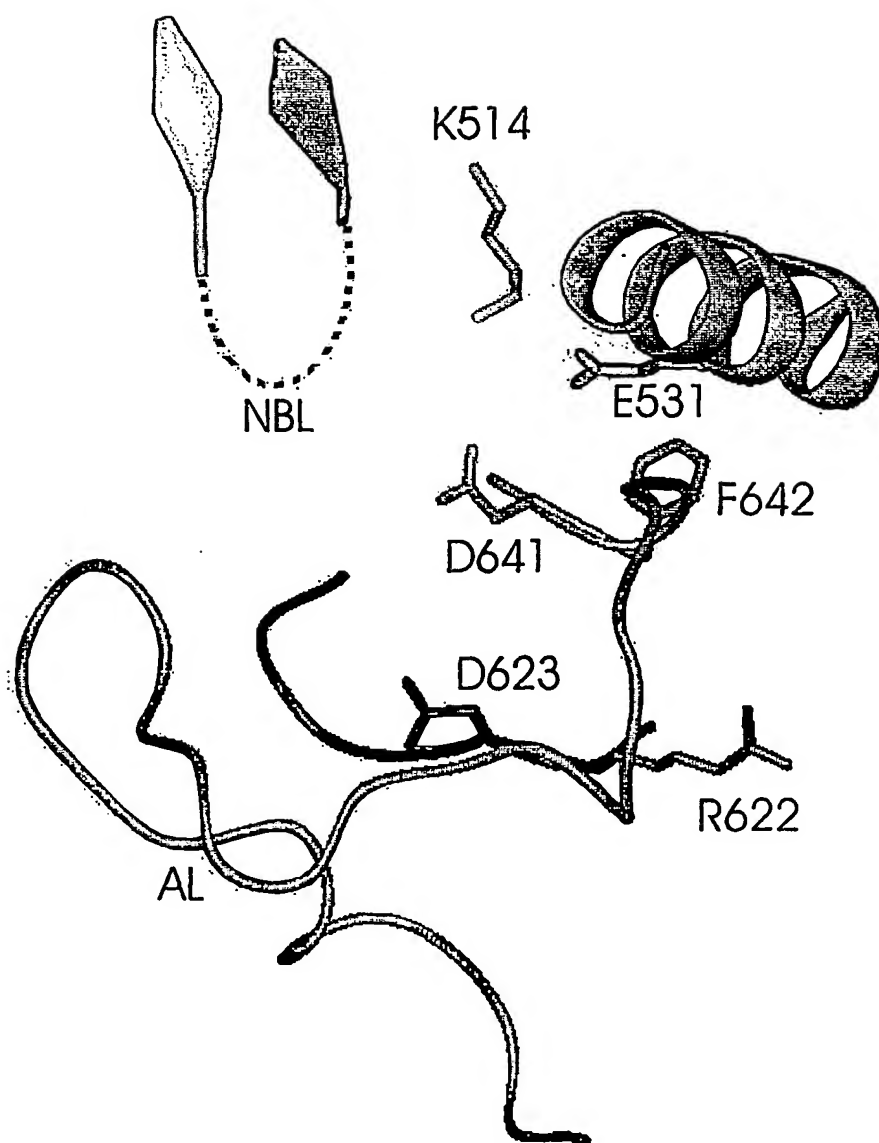
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FIG. 3B



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FIG. 3C



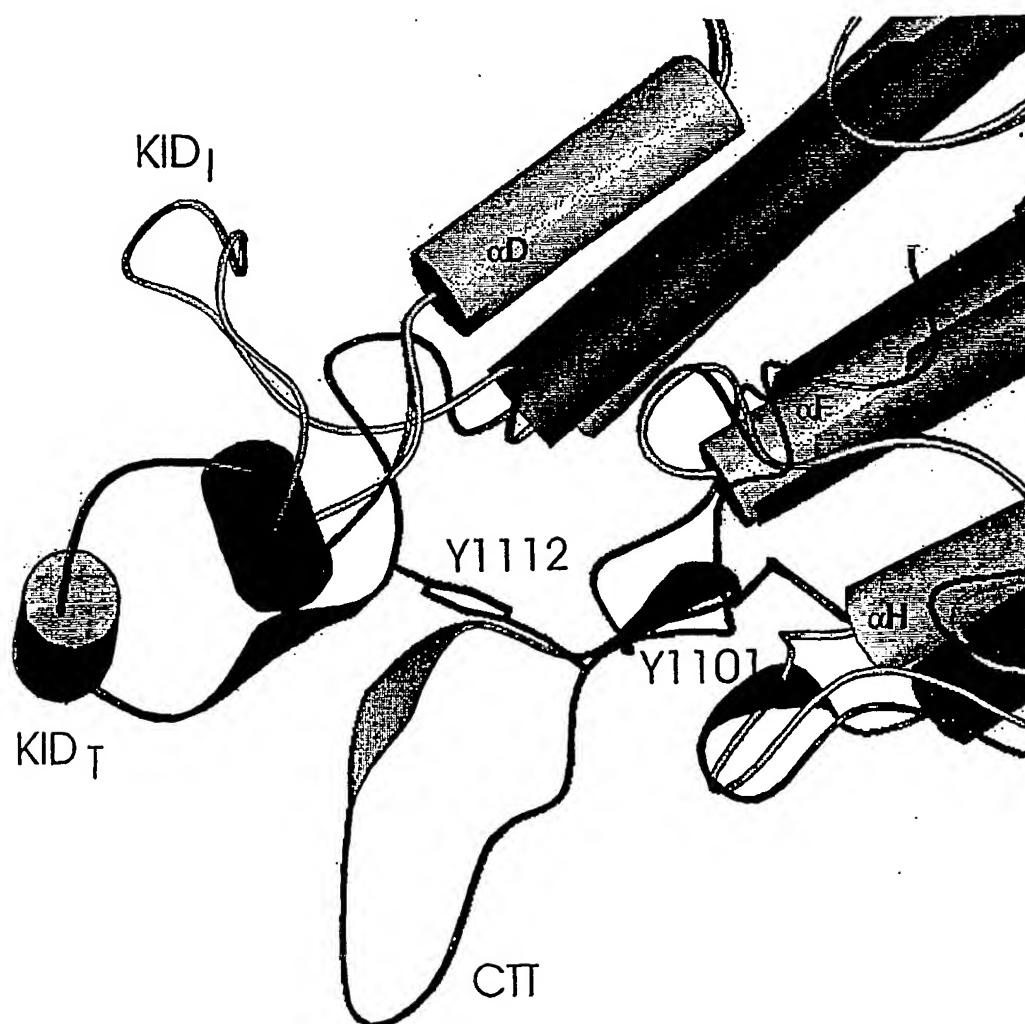
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FIG. 4



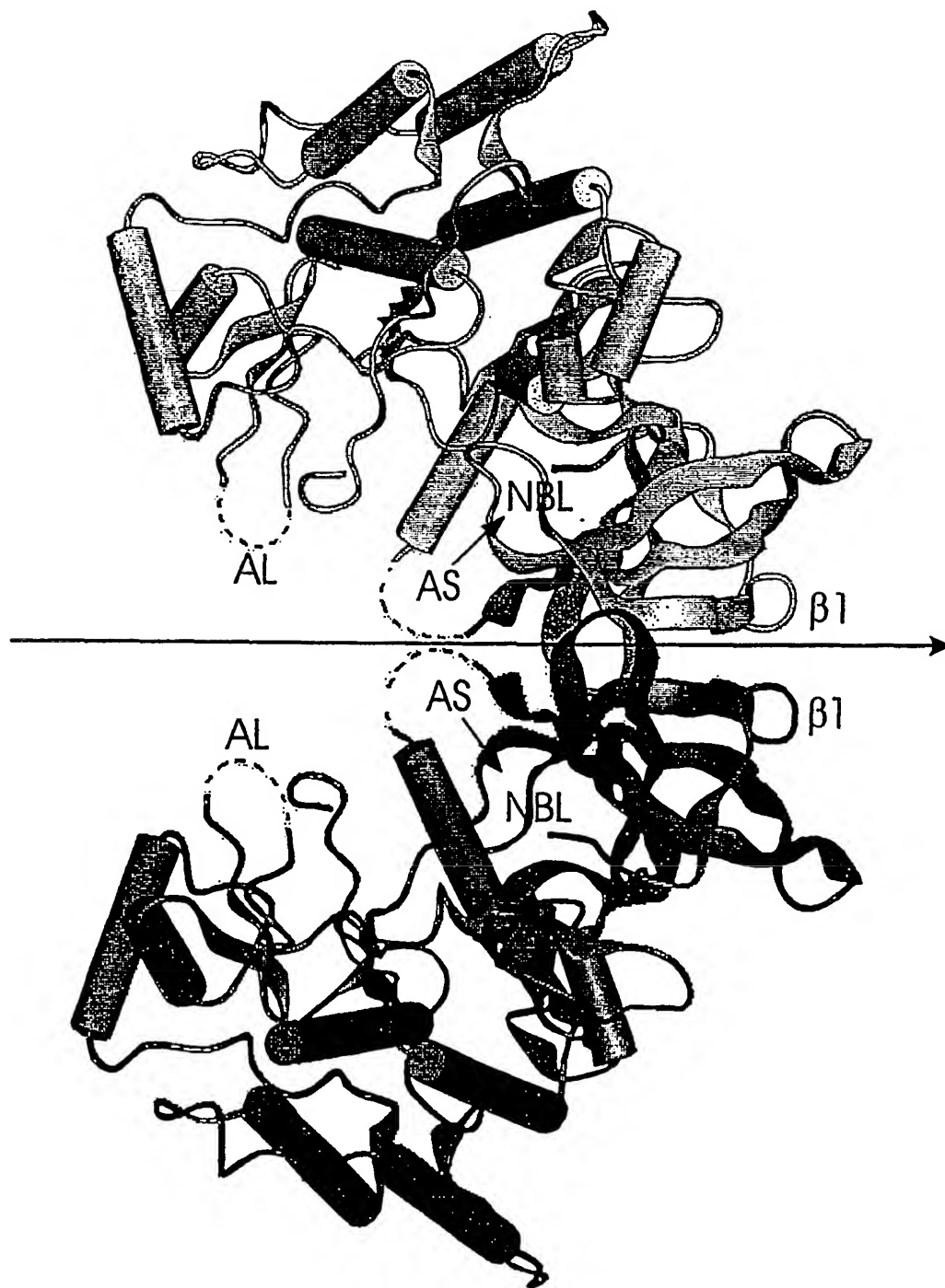
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FIG. 5



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FIG. 6



## SEQUENCE LISTING

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<120> Crystallized Cytoplasmic Tie2 Receptor Tyrosine Kinase Domain  
and Method of Determining and Designing Modulators of the Same

<130> Attorney Docket No. 4067

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2

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1 5																
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Cys	His	Glu	Asp	Thr	Gly	Glu	Cys	Ile	Cys	Pro	Pro	Gly	Phe	Met	Gly	
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Leu Pro Asp Pro Tyr Gly Cys Ser Cys Ala Thr Gly Trp Lys Gly Leu	
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cag tgc aat gaa gca tgc cac cct ggt ttt tac ggg cca gat tgt aag	1084
Gln Cys Asn Glu Ala Cys His Pro Gly Phe Tyr Gly Pro Asp Cys Lys	
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ctt agg tgc agc tgc aac aat ggg gag atg tgt gat cgc ttc caa gga	1132
Leu Arg Cys Ser Cys Asn Asn Gly Glu Met Cys Asp Arg Phe Gln Gly	
315 320 325	
tgt ctc tgc tct cca gga tgg cag ggg ctc cag tgt gag aga gaa ggc	1180
Cys Leu Cys Ser Pro Gly Trp Gln Gly Leu Gln Cys Glu Arg Glu Gly	
330 335 340	
ata ccg agg atg acc cca aag ata gtg gat ttg cca gat cat ata gaa	1228
Ile Pro Arg Met Thr Pro Lys Ile Val Asp Leu Pro Asp His Ile Glu	
345 350 355 360	
gta aac agt ggt aaa ttt aat ccc att tgc aaa gct tct ggc tgg ccg	1276
Val Asn Ser Gly Lys Phe Asn Pro Ile Cys Lys Ala Ser Gly Trp Pro	
365 370 375	
cta cct act aat gaa gaa atg acc ctg gtg aag ccg gat ggg aca gtg	1324
Leu Pro Thr Asn Glu Glu Met Thr Leu Val Lys Pro Asp Gly Thr Val	
380 385 390	
ctc cat cca aaa gac ttt aac cat acg gat cat ttc tca gta gcc ata	1372
Leu His Pro Lys Asp Phe Asn His Thr Asp His Phe Ser Val Ala Ile	
395 400 405	
ttc acc atc cac cgg atc ctc ccc cct gac tca gga gtt tgg gtc tgc	1420
Phe Thr Ile His Arg Ile Leu Pro Pro Asp Ser Gly Val Trp Val Cys	
410 415 420	
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Ser Val Asn Thr Val Ala Gly Met Val Glu Lys Pro Phe Asn Ile Ser	
425 430 435 440	
gtt aaa gtt ctt cca aag ccc ctg aat gcc cca aac gtg att gac act	1516
Val Lys Val Leu Pro Lys Pro Leu Asn Ala Pro Asn Val Ile Asp Thr	
445 450 455	
gga cat aac ttt gct gtc atc aac atc agc tct gag cct tac ttt ggg	1564
Gly His Asn Phe Ala Val Ile Asn Ile Ser Ser Glu Pro Tyr Phe Gly	
460 465 470	
gat gga cca atc aaa tcc aag aag ctt cta tac aaa ccc gtt aat cac	1612
Asp Gly Pro Ile Lys Ser Lys Lys Leu Leu Tyr Lys Pro Val Asn His	
475 480 485	
tat gag gct tgg caa cat att caa gtg aca aat gag att gtt aca ctc	1660
Tyr Glu Ala Trp Gln His Ile Gln Val Thr Asn Glu Ile Val Thr Leu	
490 495 500	
aac tat ttg gaa cct cgg aca gaa tat gaa ctc tgt gtg caa ctg gtc	1708



Asn	Tyr	Leu	Glu	Pro	Arg	Thr	Glu	Tyr	Glu	Leu	Cys	Val	Gln	Leu	Val	
505					510					515					520	
cgt	cgt	gga	gag	ggg	ggg	gaa	ggg	cat	cct	gga	cct	gtg	aga	cgc	ttc	1756
Arg	Arg	Gly	Glu	Gly	Gly	Glu	Gly	His	Pro	Gly	Pro	Val	Arg	Arg	Phe	
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aca	aca	gct	tct	atc	gga	ctc	cct	cct	cca	aga	ggg	cta	aat	ctc	ctg	1804
Thr	Thr	Ala		Ile	Gly	Leu	Pro	Pro	Pro	Arg	Gly	Leu	Asn	Leu	Leu	
				540				545					550			
cct	aaa	agt	cag	acc	act	cta	aat	ttg	acc	tgg	caa	cca	ata	ttt	cca	1852
Pro	Lys	Ser	Gln	Thr	Thr	Leu	Asn	Leu	Thr	Trp	Gln	Pro	Ile	Phe	Pro	
		555					560					565				
agc	tcg	gaa	gat	gac	ttt	tat	gtt	gaa	gtg	gag	aga	agg	tct	gtg	caa	1900
Ser	Ser	Glu	Asp	Asp	Phe	Tyr	Val	Glu	Val	Glu	Arg	Arg	Ser	Val	Gln	
		570				575						580				
aaa	agt	gat	cag	cag	aat	att	aaa	gtt	cca	ggc	aac	ttg	act	tcg	gtg	1948
Lys	Ser	Asp	Gln	Gln	Asn	Ile	Lys	Val	Pro	Gly	Asn	Leu	Thr	Ser	Val	
585					590					595					600	
cta	ctt	aac	aac	tta	cat	ccc	agg	gag	cag	tac	gtg	gtc	cga	gct	aga	1996
Leu	Leu	Asn	Asn	Leu	His	Pro	Arg	Glu	Gln	Tyr	Val	Val	Arg	Ala	Arg	
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gtc	aac	acc	aag	gcc	cag	ggg	gaa	tgg	agt	gaa	gat	ctc	act	gct	tgg	2044
Val	Asn	Thr		Lys	Ala	Gln	Gly	Glu	Trp	Ser	Glu	Asp	Leu	Thr	Ala	Trp
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acc	ctt	agt	gac	att	ctt	cct	cct	caa	cca	gaa	aac	atc	aag	att	tcc	2092
Thr	Leu	Ser	Asp	Ile	Leu	Pro	Pro	Gln	Pro	Glu	Asn	Ile	Lys	Ile	Ser	
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Asn	Ile	Thr	His	Ser	Ser	Ala	Val	Ile	Ser	Trp	Thr	Ile	Leu	Asp	Gly	
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Tyr	Ser	Ile	Ser	Ser	Ile	Thr	Ile	Arg	Tyr	Lys	Val	Gln	Gly	Lys	Asn	
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gaa	gac	cag	cac	gtt	gat	gtg	aag	ata	aag	aat	gcc	acc	atc	att	cag	2236
Glu	Asp	Gln	His	Val	Asp	Val	Lys	Ile	Lys	Asn	Ala	Thr	Ile	Ile	Gln	
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tat	cag	ctc	aag	ggc	cta	gag	cct	gaa	aca	gca	tac	cag	gtg	gac	att	2284
Tyr	Gln	Leu	Lys	Gly	Leu	Glu	Pro	Glu	Thr	Ala	Tyr	Gln	Val	Asp	Ile	
			700					705					710			
ttt	gca	gag	aac	aac	ata	ggg	tca	agc	aac	cca	gcc	ttt	tct	cat	gaa	2332
Phe	Ala	Glu	Asn	Asn	Ile	Gly	Ser	Ser	Asn	Pro	Ala	Phe	Ser	His	Glu	
		715					720					725				
ctg	gtg	acc	ctc	cca	gaa	tct	caa	gca	cca	gcg	gac	ctc	gga	ggg	ggg	2380
Leu	Val	Thr	Leu	Pro	Glu	Ser	Gln	Ala	Pro	Ala	Asp	Leu	Gly	Gly	Gly	
		730				735					740					
aag	atg	ctg	ctt	ata	gcc	atc	ctt	ggc	tct	gct	gga	atg	acc	tgc	ctg	2428
Lys	Met	Leu	Leu	Ile	Ala	Ile	Leu	Gly	Ser	Ala	Gly	Met	Thr	Cys	Leu	
745					750				755						760	
act	gtg	ctg	ttg	gcc	ttt	ctg	atc	ata	ttg	caa	ttg	aag	agg	gca	aat	2476
Thr	Val	Leu	Leu	Ala	Phe	Leu	Ile	Ile	Leu	Gln	Leu	Lys	Arg	Ala	Asn	

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gct gtg cag ttc aac tca ggg act ctg gcc cta aac agg aag gtc aaa Ala Val Gln Phe Asn Ser Gly Thr Leu Ala Leu Asn Arg Lys Val Lys 795 800 805			2572
aac aac cca gat cct aca att tat cca gtg ctt gac tgg aat gac atc Asn Asn Pro Asp Pro Thr Ile Tyr Pro Val Leu Asp Trp Asn Asp Ile 810 815 820			2620
aaa ttt caa gat gtg att ggg gag ggc aat ttt ggc caa gtt ctt aag Lys Phe Gln Asp Val Ile Gly Glu Gly Asn Phe Gly Gln Val Leu Lys 825 830 835 840			2668
gcg cgc atc aag aag gat ggg tta cgg atg gat gct gcc atc aaa aga Ala Arg Ile Lys Lys Asp Gly Leu Arg Met Asp Ala Ala Ile Lys Arg 845 850 855			2716
atg aaa gaa tat gcc tcc aaa gat gat cac agg gac ttt gca gga gaa Met Lys Glu Tyr Ala Ser Lys Asp Asp His Arg Asp Phe Ala Gly Glu 860 865 870			2764
ctg gaa gtt ctt tgt aaa ctt gga cac cat cca aac atc atc aat ctc Leu Glu Val Leu Cys Lys Leu Gly His His Pro Asn Ile Ile Asn Leu 875 880 885			2812
tta gga gca tgt gaa cat cga ggc tac ttg tac ctg gcc att gag tac Leu Gly Ala Cys Glu His Arg Gly Tyr Leu Tyr Leu Ala Ile Glu Tyr 890 895 900			2860
gcg ccc cat gga aac ctt ctg gac ttc ctt cgc aag agc cgt gtg ctg Ala Pro His Gly Asn Leu Leu Asp Phe Leu Arg Lys Ser Arg Val Leu 905 910 915 920			2908
gag acg gac cca gca ttt gcc att gcc aat agc acc gcg tcc aca ctg Glu Thr Asp Pro Ala Phe Ala Ile Ala Asn Ser Thr Ala Ser Thr Leu 925 930 935			2956
tcc tcc cag cag ctc ctt cac ttc gct gcc gac gtg gcc cgg ggc atg Ser Ser Gln Gln Leu Leu His Phe Ala Ala Asp Val Ala Arg Gly Met 940 945 950			3004
gac tac ttg agc caa aaa cag ttt atc cac agg gat ctg gct gcc aga Asp Tyr Leu Ser Gln Lys Gln Phe Ile His Arg Asp Leu Ala Ala Arg 955 960 965			3052
aac att tta gtt ggt gaa aac tat gtg gca aaa ata gca gat ttt gga Asn Ile Leu Val Gly Glu Asn Tyr Val Ala Lys Ile Ala Asp Phe Gly 970 975 980			3100
ttg tcc cga ggt caa gag gtg tac gtg aaa aag aca atg gga agg ctc Leu Ser Arg Gly Gln Glu Val Tyr Val Lys Lys Thr Met Gly Arg Leu 985 990 995 1000			3148
cca gtg cgc tgg atg gcc atc gag tca ctg aat tac agt gtg tac Pro Val Arg Trp Met Ala Ile Glu Ser Leu Asn Tyr Ser Val Tyr 1005 1010 1015			3193
aca acc aac agt gat gta tgg tcc tat ggt gtg tta cta tgg gag Thr Thr Asn Ser Asp Val Trp Ser Tyr Gly Val Leu Leu Trp Glu 1020 1025 1030			3238

6

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gaa ctc tac gag aag ctg ccc cag ggc tac aga ctg gag aag ccc      3328
Glu Leu Tyr Glu Lys Leu Pro Gln Gly Tyr Arg Leu Glu Lys Pro
      1050      1055      1060

ctg aac tgt gat gat gag gtg tat gat cta atg aga caa tgc tgg      3373
Leu Asn Cys Asp Asp Glu Val Tyr Asp Leu Met Arg Gln Cys Trp
      1065      1070      1075

cgg gag aag cct tat gag agg cca tca ttt gcc cag ata ttg gtg      3418
Arg Glu Lys Pro Tyr Glu Arg Pro Ser Phe Ala Gln Ile Leu Val
      1080      1085      1090

tcc tta aac aga atg tta gag gag cga aag acc tac gtg aat acc      3463
Ser Leu Asn Arg Met Leu Glu Glu Arg Lys Thr Tyr Val Asn Thr
      1095      1100      1105

acg ctt tat gag aag ttt act tat gca gga att gac tgt tct gct      3508
Thr Leu Tyr Glu Lys Phe Thr Tyr Ala Gly Ile Asp Cys Ser Ala
      1110      1115      1120

gaa gaa gcg gcc tag gacagaacat ctgtataccc tctgtttccc tttcactggc      3563
Glu Glu Ala Ala

atgggagacc cttgacaact gctgagaaaa catgcctctg ccaaaggatg tgatatataa      3623

gtgtacatat gtgctggaat tctaacaagt cataggttaa tatttaagac actgaaaaat      3683

ctaagtgata taaatcagat tcttctctct cattttatcc ctcacctgta gcatgccagt      3743

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ccaggatgct aacatctaaa aatagactta aatctcattg ettacaagcc taagaatctt      3863

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gacatttata tattgaatta atatccctac atgtattgca cattgtaaaa agtttttagtt      4043

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<211> 1124

<212> PRT

<213> Homo sapiens

<400> 2

Met Asp Ser Leu Ala Ser Leu Val Leu Cys Gly Val Ser Leu Leu Leu

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7

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	20	25	30
Pro Leu Val	Ser Asp Ala	Glu Thr Ser	Leu Thr Cys Ile Ala Ser Gly
	35	40	45
Trp Arg Pro	His Glu Pro	Ile Thr Ile	Gly Arg Asp Phe Glu Ala Leu
	50	55	60
Met Asn Gln	His Gln Asp	Pro Leu Glu	Val Thr Gln Asp Val Thr Arg
65	70	75	80
Glu Trp Ala	Lys Lys Val	Val Trp Lys	Arg Glu Lys Ala Ser Lys Ile
	85	90	95
Asn Gly Ala	Tyr Phe Cys	Glu Gly Arg	Val Arg Gly Glu Ala Ile Arg
	100	105	110
Ile Arg Thr	Met Lys Met	Arg Gln Gln	Ala Ser Phe Leu Pro Ala Thr
	115	120	125
Leu Thr Met	Thr Val Asp	Lys Gly Asp	Asn Val Asn Ile Ser Phe Lys
	130	135	140
Lys Val Leu	Ile Lys Glu	Glu Asp Ala	Val Ile Tyr Lys Asn Gly Ser
145	150	155	160
Phe Ile His	Ser Val Pro	Arg His Glu	Val Pro Asp Ile Leu Glu Val
	165	170	175
His Leu Pro	His Ala Gln	Pro Gln Asp	Ala Gly Val Tyr Ser Ala Arg
	180	185	190
Tyr Ile Gly	Gly Asn Leu	Phe Thr Ser	Ala Phe Thr Arg Leu Ile Val
	195	200	205
Arg Arg Cys	Glu Ala Gln	Lys Trp Gly	Pro Glu Cys Asn His Leu Cys
	210	215	220
Thr Ala Cys	Met Asn Asn	Gly Val Cys	His Glu Asp Thr Gly Glu Cys
225	230	235	240

Ile Cys Pro Pro Gly Phe Met Gly Arg Thr Cys Glu Lys Ala Cys Glu  
 245 250 255

Leu His Thr Phe Gly Arg Thr Cys Lys Glu Arg Cys Ser Gly Gln Glu  
 260 265 270

Gly Cys Lys Ser Tyr Val Phe Cys Leu Pro Asp Pro Tyr Gly Cys Ser  
 275 280 285

Cys Ala Thr Gly Trp Lys Gly Leu Gln Cys Asn Glu Ala Cys His Pro  
 290 295 300

Gly Phe Tyr Gly Pro Asp Cys Lys Leu Arg Cys Ser Cys Asn Asn Gly  
 305 310 315 320

Glu Met Cys Asp Arg Phe Gln Gly Cys Leu Cys Ser Pro Gly Trp Gln  
 325 330 335

Gly Leu Gln Cys Glu Arg Glu Gly Ile Pro Arg Met Thr Pro Lys Ile  
 340 345 350

Val Asp Leu Pro Asp His Ile Glu Val Asn Ser Gly Lys Phe Asn Pro  
 355 360 365

Ile Cys Lys Ala Ser Gly Trp Pro Leu Pro Thr Asn Glu Glu Met Thr  
 370 375 380

Leu Val Lys Pro Asp Gly Thr Val Leu His Pro Lys Asp Phe Asn His  
 385 390 395 400

Thr Asp His Phe Ser Val Ala Ile Phe Thr Ile His Arg Ile Leu Pro  
 405 410 415

Pro Asp Ser Gly Val Trp Val Cys Ser Val Asn Thr Val Ala Gly Met  
 420 425 430

Val Glu Lys Pro Phe Asn Ile Ser Val Lys Val Leu Pro Lys Pro Leu  
 435 440 445

Asn Ala Pro Asn Val Ile Asp Thr Gly His Asn Phe Ala Val Ile Asn  
 450 455 460

Ile Ser Ser Glu Pro Tyr Phe Gly Asp Gly Pro Ile Lys Ser Lys Lys  
 465 470 475 480

Leu Leu Tyr Lys Pro Val Asn His Tyr Glu Ala Trp Gln His Ile Gln  
 485 490 495

Val Thr Asn Glu Ile Val Thr Leu Asn Tyr Leu Glu Pro Arg Thr Glu  
 500 505 510

Tyr Glu Leu Cys Val Gln Leu Val Arg Arg Gly Glu Gly Gly Glu Gly  
 515 520 525

His Pro Gly Pro Val Arg Arg Phe Thr Thr Ala Ser Ile Gly Leu Pro  
 530 535 540

Pro Pro Arg Gly Leu Asn Leu Leu Pro Lys Ser Gln Thr Thr Leu Asn  
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Leu Thr Trp Gln Pro Ile Phe Pro Ser Ser Glu Asp Asp Phe Tyr Val  
 565 570 575

Glu Val Glu Arg Arg Ser Val Gln Lys Ser Asp Gln Gln Asn Ile Lys  
 580 585 590

Val Pro Gly Asn Leu Thr Ser Val Leu Leu Asn Asn Leu His Pro Arg  
 595 600 605

Glu Gln Tyr Val Val Arg Ala Arg Val Asn Thr Lys Ala Gln Gly Glu  
 610 615 620

Trp Ser Glu Asp Leu Thr Ala Trp Thr Leu Ser Asp Ile Leu Pro Pro  
 625 630 635 640

Gln Pro Glu Asn Ile Lys Ile Ser Asn Ile Thr His Ser Ser Ala Val  
 645 650 655

Ile Ser Trp Thr Ile Leu Asp Gly Tyr Ser Ile Ser Ser Ile Thr Ile  
 660 665 670

Arg Tyr Lys Val Gln Gly Lys Asn Glu Asp Gln His Val Asp Val Lys  
 675 680 685

Ile Lys Asn Ala Thr Ile Ile Gln Tyr Gln Leu Lys Gly Leu Glu Pro

10

690	695	700
Glu Thr Ala Tyr Gln Val Asp Ile Phe Ala Glu Asn Asn Ile Gly Ser		
705	710	715 720
Ser Asn Pro Ala Phe Ser His Glu Leu Val Thr Leu Pro Glu Ser Gln		
	725	730 735
Ala Pro Ala Asp Leu Gly Gly Gly Lys Met Leu Leu Ile Ala Ile Leu		
	740	745 750
Gly Ser Ala Gly Met Thr Cys Leu Thr Val Leu Leu Ala Phe Leu Ile		
	755	760 765
Ile Leu Gln Leu Lys Arg Ala Asn Val Gln Arg Arg Met Ala Gln Ala		
	770	775 780
Phe Gln Asn Val Arg Glu Glu Pro Ala Val Gln Phe Asn Ser Gly Thr		
	785	790 795 800
Leu Ala Leu Asn Arg Lys Val Lys Asn Asn Pro Asp Pro Thr Ile Tyr		
	805	810 815
Pro Val Leu Asp Trp Asn Asp Ile Lys Phe Gln Asp Val Ile Gly Glu		
	820	825 830
Gly Asn Phe Gly Gln Val Leu Lys Ala Arg Ile Lys Lys Asp Gly Leu		
	835	840 845
Arg Met Asp Ala Ala Ile Lys Arg Met Lys Glu Tyr Ala Ser Lys Asp		
	850	855 860
Asp His Arg Asp Phe Ala Gly Glu Leu Glu Val Leu Cys Lys Leu Gly		
	865	870 875 880
His His Pro Asn Ile Ile Asn Leu Leu Gly Ala Cys Glu His Arg Gly		
	885	890 895
Tyr Leu Tyr Leu Ala Ile Glu Tyr Ala Pro His Gly Asn Leu Leu Asp		
	900	905 910
Phe Leu Arg Lys Ser Arg Val Leu Glu Thr Asp Pro Ala Phe Ala Ile		
	915	920 925

Ala Asn Ser Thr Ala Ser Thr Leu Ser Ser Gln Gln Leu Leu His Phe  
 930 935 940

Ala Ala Asp Val Ala Arg Gly Met Asp Tyr Leu Ser Gln Lys Gln Phe  
 945 950 955 960

Ile His Arg Asp Leu Ala Ala Arg Asn Ile Leu Val Gly Glu Asn Tyr  
 965 970 975

Val Ala Lys Ile Ala Asp Phe Gly Leu Ser Arg Gly Gln Glu Val Tyr  
 980 985 990

Val Lys Lys Thr Met Gly Arg Leu Pro Val Arg Trp Met Ala Ile Glu  
 995 1000 1005

Ser Leu Asn Tyr Ser Val Tyr Thr Thr Asn Ser Asp Val Trp Ser  
 1010 1015 1020

Tyr Gly Val Leu Leu Trp Glu Ile Val Ser Leu Gly Gly Thr Pro  
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Tyr Cys Gly Met Thr Cys Ala Glu Leu Tyr Glu Lys Leu Pro Gln  
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Gly Tyr Arg Leu Glu Lys Pro Leu Asn Cys Asp Asp Glu Val Tyr  
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Asp Leu Met Arg Gln Cys Trp Arg Glu Lys Pro Tyr Glu Arg Pro  
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Ser Phe Ala Gln Ile Leu Val Ser Leu Asn Arg Met Leu Glu Glu  
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 1100 1105 1110

Ala Gly Ile Asp Cys Ser Ala Glu Glu Ala Ala  
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12

&lt;211&gt; 984

&lt;212&gt; DNA

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Thr Ile Tyr Pro Val Leu Asp Trp Asn Asp Ile Lys Phe Gln Asp Val	
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Ile Gly Glu Gly Asn Phe Gly Gln Val Leu Lys Ala Arg Ile Lys Lys	
35 40 45	
gat ggg tta cgg atg gat gct gcc atc aaa aga atg aaa gaa tat gcc	192
Asp Gly Leu Arg Met Asp Ala Ala Ile Lys Arg Met Lys Glu Tyr Ala	
50 55 60	
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Ser Lys Asp Asp His Arg Asp Phe Ala Gly Glu Leu Glu Val Leu Cys	
65 70 75 80	
aaa ctt gga cac cat cca aac atc atc aat ctc tta gga gca tgt gaa	288
Lys Leu Gly His His Pro Asn Ile Ile Asn Leu Leu Gly Ala Cys Glu	
85 90 95	
cat cga ggc tac ttg tac ctg gcc att gag tac gcg ccc cat gga aac	336
His Arg Gly Tyr Leu Tyr Leu Ala Ile Glu Tyr Ala Pro His Gly Asn	
100 105 110	
ctt ctg gac ttc ctt cgc aag agc cgt gtg ctg gag acg gac cca gca	384
Leu Leu Asp Phe Leu Arg Lys Ser Arg Val Leu Glu Thr Asp Pro Ala	
115 120 125	
ttt gcc att gcc aat agc acc gcg tcc aca ctg tcc tcc cag cag ctc	432
Phe Ala Ile Ala Asn Ser Thr Ala Ser Thr Leu Ser Ser Gln Gln Leu	
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Leu His Phe Ala Ala Asp Val Ala Arg Gly Met Asp Tyr Leu Ser Gln	
145 150 155 160	
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Lys Gln Phe Ile His Arg Asp Leu Ala Ala Arg Asn Ile Leu Val Gly	

13

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gag	gtg	tat	gtg	aaa	aag	aca	atg	gga	agg	ctc	cca	gtg	cgc	tgg	atg	624					
Glu	Val	Tyr	Val	Lys	Lys	Thr	Met	Gly	Arg	Leu	Pro	Val	Arg	Trp	Met						
195										200					205						
gcc	atc	gag	tca	ctg	aat	tac	agt	gtg	tac	aca	acc	aac	agt	gat	gta	672					
Ala	Ile	Glu	Ser	Leu	Asn	Tyr	Ser	Val	Tyr	Thr	Thr	Asn	Ser	Asp	Val						
210										215					220						
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Trp	Ser	Tyr	Gly	Val	Leu	Leu	Trp	Glu	Ile	Val	Ser	Leu	Gly	Gly	Thr						
225										230					235					240	
ccc	tac	tgc	gga	atg	act	tgt	gca	gaa	ctc	tac	gag	aag	ctg	ccc	cag	768					
Pro	Tyr	Cys	Gly	Met	Thr	Cys	Ala	Glu	Leu	Tyr	Glu	Lys	Leu	Pro	Gln						
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Gly	Tyr	Arg	Leu	Glu	Lys	Pro	Leu	Asn	Cys	Asp	Asp	Glu	Val	Tyr	Asp						
260										265					270						
cta	atg	aga	caa	tgc	tgg	cgg	gag	aag	cct	tat	gag	agg	cca	tca	ttt	864					
Leu	Met	Arg	Gln	Cys	Trp	Arg	Glu	Lys	Pro	Tyr	Glu	Arg	Pro	Ser	Phe						
275										280					285						
gcc	cag	ata	ttg	gtg	tcc	tta	aac	aga	atg	tta	gag	gag	cga	aag	acc	912					
Ala	Gln	Ile	Leu	Val	Ser	Leu	Asn	Arg	Met	Leu	Glu	Glu	Arg	Lys	Thr						
290										295					300						
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Tyr	Val	Asn	Thr	Thr	Leu	Tyr	Glu	Lys	Phe	Thr	Tyr	Ala	Gly	Ile	Asp						
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14

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Asp Gly Leu Arg Met Asp Ala Ala Ile Lys Arg Met Lys Glu Tyr Ala	50		55		60
Ser Lys Asp Asp His Arg Asp Phe Ala Gly Glu Leu Glu Val Leu Cys	65		70		75
Lys Leu Gly His His Pro Asn Ile Ile Asn Leu Leu Gly Ala Cys Glu		85		90	95
His Arg Gly Tyr Leu Tyr Leu Ala Ile Glu Tyr Ala Pro His Gly Asn		100		105	110
Leu Leu Asp Phe Leu Arg Lys Ser Arg Val Leu Glu Thr Asp Pro Ala		115		120	125
Phe Ala Ile Ala Asn Ser Thr Ala Ser Thr Leu Ser Ser Gln Gln Leu		130		135	140
Leu His Phe Ala Ala Asp Val Ala Arg Gly Met Asp Tyr Leu Ser Gln		145		150	155
Lys Gln Phe Ile His Arg Asp Leu Ala Ala Arg Asn Ile Leu Val Gly		165		170	175
Glu Asn Tyr Val Ala Lys Ile Ala Asp Phe Gly Leu Ser Arg Gly Gln		180		185	190
Glu Val Tyr Val Lys Lys Thr Met Gly Arg Leu Pro Val Arg Trp Met		195		200	205
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Trp Ser Tyr Gly Val Leu Leu Trp Glu Ile Val Ser Leu Gly Gly Thr		225		230	235
Pro Tyr Cys Gly Met Thr Cys Ala Glu Leu Tyr Glu Lys Leu Pro Gln		245		250	255

Gly Tyr Arg Leu Glu Lys Pro Leu Asn Cys Asp Asp Glu Val Tyr Asp  
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 Thr Ile Tyr Pro Val Leu Asp Trp Asn Asp Ile Lys Phe Gln Asp Val  
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gat ggg tta cgg atg gat gct gcc atc aaa aga atg aaa gaa tat gcc 192  
 Asp Gly Leu Arg Met Asp Ala Ala Ile Lys Arg Met Lys Glu Tyr Ala  
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 Ser Lys Asp Asp His Arg Asp Phe Ala Gly Glu Leu Glu Val Leu Cys

16

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Lys Leu Gly His His 85	Pro Asn Ile Ile 90	Leu Leu Gly Ala Cys Glu 95		
cat cga ggc ttc ttg tac ctg gcc att gag tac gcg ccc cat gga aac				336
His Arg Gly Phe Leu Tyr Leu Ala Ile 105	Glu Tyr Ala Pro His Gly Asn 110			
ctt ctg gac ttc ctt cgc aag agc cgt gtg ctg gag acg gac cca gca				384
Leu Leu Asp Phe Leu Arg Lys Ser Arg Val Leu Glu Thr Asp Pro Ala 115	120	125		
ttt gcc att gcc aat agc acc gcg tcc aca ctg tcc tcc cag cag ctc				432
Phe Ala Ile Ala Asn Ser Thr Ala Ser Thr Leu Ser Ser Gln Gln Leu 130	135	140		
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Leu His Phe Ala Ala Asp Val Ala Arg Gly Met Asp Tyr Leu Ser Gln 145	150	155	160	
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Lys Gln Phe Ile His Arg Asp Leu Ala Ala Arg Asn Ile Leu Val Gly 165	170	175		
gaa aac tat gtg gca aaa ata gca gat ttt gga ttg tcc cga ggt caa				576
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gag gtg tat gtg aaa aag aca atg gga agg ctc cca gtg cgc tgg atg				624
Glu Val Tyr Val Lys Lys Thr Met Gly Arg Leu Pro Val Arg Trp Met 195	200	205		
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Trp Ser Tyr Gly Val Leu Leu Trp Glu Ile Val Ser Leu Gly Gly Thr 225	230	235	240	
ccc tac tgc gga atg act tgt gca gaa ctc ttc gag aag ctg ccc cag				768
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Gly Tyr Arg Leu Glu Lys Pro Leu Asn Cys Asp Asp Glu Val Tyr Asp 260	265	270		
cta atg aga caa tgc tgg cgg gag aag cct tat gag agg cca tca ttt				864
Leu Met Arg Gln Cys Trp Arg Glu Lys Pro Tyr Glu Arg Pro Ser Phe 275	280	285		
gcc cag ata ttg gtg tcc tta aac aga atg tta gag gag cga aag acc				912
Ala Gln Ile Leu Val Ser Leu Asn Arg Met Leu Glu Glu Arg Lys Thr 290	295	300		
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Tyr Val Asn Thr Thr Leu Tyr Glu Lys Phe Thr Tyr Ala Gly Ile Asp 305	310	315	320	
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Cys Ala Ala Glu Glu Ala Ala				

17

325

&lt;210&gt; 6

&lt;211&gt; 327

&lt;212&gt; PRT

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&lt;400&gt; 6

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Thr Ile Tyr Pro Val Leu Asp Trp Asn Asp Ile Lys Phe Gln Asp Val  
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Ile Gly Glu Gly Asn Phe Gly Gln Val Leu Lys Ala Arg Ile Lys Lys  
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&lt;309&gt; 1997-07-23

&lt;313&gt; (491) .. (500)

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&lt;309&gt; 1997-07-23

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&lt;400&gt; 9

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          20           25           30
Ile Gly Lys His Lys Asn Ile Ile Asn Leu Leu Gly Ala Cys Thr Gln
          35           40           45
Asp Gly Pro Leu Tyr Val Ile Val Glu Tyr Ala Ser Lys Gly Asn Leu
          50           55           60
Arg Glu Tyr Leu Gln Ala Arg Arg Pro
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&lt;212&gt; PRT

&lt;213&gt; Homo sapiens

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&lt;309&gt; 1997-07-23

&lt;313&gt; (592) .. (647)

&lt;400&gt; 10

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Ala Asp Phe Gly Leu Ala Arg Asp
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&lt;213&gt; Homo sapiens

&lt;300&gt;

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&lt;309&gt; 1997-07-23

&lt;313&gt; (651) .. (761)

&lt;400&gt; 11

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			20					25					30		
Val	Trp	Ser	Phe	Gly	Val	Leu	Leu	Trp	Glu	Ile	Phe	Thr	Leu	Gly	Gly
		35					40					45			
Ser	Pro	Tyr	Pro	Gly	Val	Pro	Val	Glu	Glu	Leu	Phe	Lys	Leu	Leu	Lys
	50					55					60				
Glu	Gly	His	Arg	Met	Asp	Lys	Pro	Ser	Asn	Cys	Thr	Asn	Glu	Leu	Tyr
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Met	Met	Met	Arg	Asp	Cys	Trp	His	Ala	Val	Pro	Ser	Gln	Arg	Pro	Thr
			85						90					95	
Phe	Lys	Gln	Leu	Val	Glu	Asp	Leu	Asp	Arg	Ile	Val	Ala	Leu	Thr	
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&lt;211&gt; 7

&lt;212&gt; PRT

&lt;213&gt; Homo sapiens

&lt;400&gt; 12

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&lt;211&gt; 17

22

&lt;212&gt; PRT

&lt;213&gt; Homo sapiens

&lt;400&gt; 13

Leu	Glu	Ala	Arg	Leu	Val	Ala	Tyr	Glu	Gly	Trp	Val	Ala	Gly	Lys	Lys
1				5					10					15	

Lys

(19) World Intellectual Property Organization  
International Bureau



(43) International Publication Date  
14 March 2002 (14.03.2002)

PCT

(10) International Publication Number  
**WO 02/020734 A3**

(51) International Patent Classification<sup>7</sup>: **C07K 14/71**,  
G06F 17/50

(21) International Application Number: PCT/US01/27486

(22) International Filing Date:  
6 September 2001 (06.09.2001)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:  
60/231,398 8 September 2000 (08.09.2000) US

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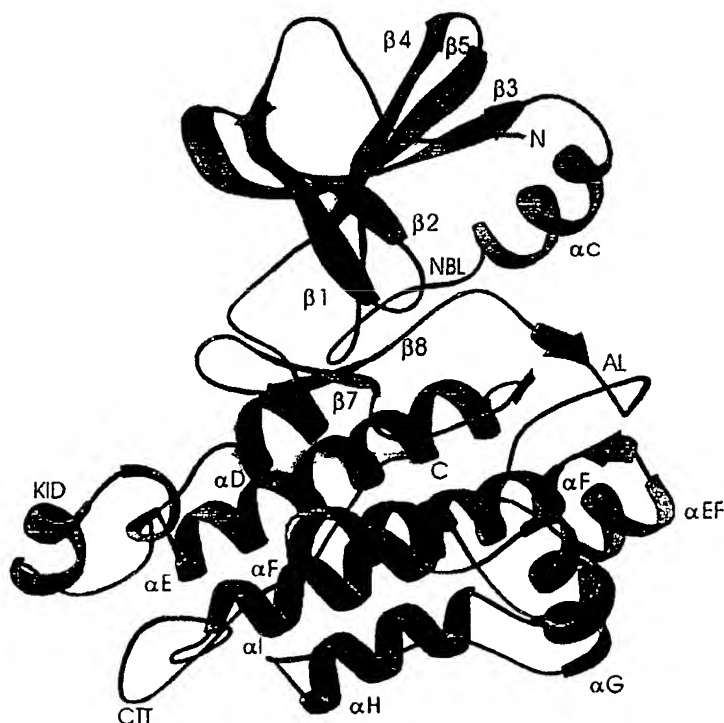
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27709 (US).

(81) Designated States (national): AE, AG, AL, AM, AT, AU,  
AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU,  
CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,  
GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,

[Continued on next page]

(54) Title: CRYSTALLIZED CYTOPLASMIC TIE2 RECEPTOR TYROSINE KINASE DOMAIN AND METHOD OF DETERMINING AND DESIGNING MODULATORS OF THE SAME



(57) Abstract: A solved three-dimensional crystal structure of a cytoplasmic Tie2 receptor tyrosine kinase domain is disclosed, along with four crystal forms of the cytoplasmic Tie2 receptor tyrosine kinase domain. The crystal forms include non- and monophosphorylated forms of the cytoplasmic Tie2 receptor tyrosine kinase domain. Methods of designing modulators of the biological activity of the cytoplasmic Tie2 receptor tyrosine kinase domain are also disclosed.



IK, IR, IS, IT, IU, IV, MA, MD, MG, MK, MN, MW,  
MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI,  
SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU,  
ZA, ZW.

Published:

*with international search report*

(84) Designated States (*regional*): ARIPO patent (GH, GM, KH, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

(88) Date of publication of the international search report:

19 June 2003

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## INTERNATIONAL SEARCH REPORT

International Application No.

PCT/US 01/27486

## A. CLASSIFICATION OF SUBJECT MATTER

IPC 7 C07K14/71 G06F17/50

According to International Patent Classification (IPC) or to both national classification and IPC

## B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

IPC 7 C07K G06F

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

EPO-Internal, WPI Data, BIOSIS, CHEM ABS Data

## C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Y	<p>WO 95 13387 A (MAX PLANCK GESELLSCHAFT) 18 May 1995 (1995-05-18)</p> <p>* See Fig 3 (TEK) and page 4 (Fig. 3); TEK = 1124 aa -&gt; identical with SEQ.ID.No 2 / APPL); and page 36, line 25 - page 37, line 27 *</p> <p style="text-align: center;">--- -/--</p>	<p>1,3-5,7, 8,13,14, 17-21, 25, 27-30, 34-41, 45,46</p>



Further documents are listed in the continuation of box C.



Patent family members are listed in annex.

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\*G\* document member of the same patent family

Date of the actual completion of the international search

14 November 2002

Date of mailing of the international search report

29/11/2002

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## INTERNATIONAL SEARCH REPORT

Int. nat. Application No.

PCT/US 01/27486

## C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Y	<p>MOHAMMADI ET AL: "Structure of the FGF receptor tyrosine kinase domain reveals a novel autoinhibitory mechanism" CELL, vol. 86, 1996, pages 577-587, XP002219716 cited in the application</p> <p>* See page 577 (introduction), page 586 (Crystallization and data collection); compare page 32 of the Description *</p>	<p>1,3-5,7, 8,13,14, 17-21, 25, 27-30, 34-41, 45,46</p>
A	<p>CALVERT: "Allelic and locus heterogeneity in inherited venous malformations" HUMAN MOLECULAR GENETICS, vol. 8, 1999, pages 1279-1289, XP002219717 * See the Abstract -&gt; Y897S *</p>	42
A	<p>ROBERTSON ET AL: "RTK mutations and human syndromes when good receptors turn bad" TIG, vol. 16, June 2000 (2000-06), pages 265-271, XP004200112 * See page 266 (Figure 1 -&gt; Tie2) and page 268 (Tyrosine kinase with Ig and EGF (TIE) family: Tie2) *</p>	1-52
A	<p>HIMANEN ET AL: "Crystal structure of the ligand-binding domain of the receptor tyrosine kinase EphB2" NATURE, vol. 396, 3 December 1998 (1998-12-03), pages 486-491, XP002134939 ISSN: 0028-0836 * See page 486 (Summary) and page 490 (Methods) *</p>	1-52
A	<p>DJORDJEVIC: "Crystallization and preliminary x-ray studies of NADPH-cytochrome P450 reductase" PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES, USA, vol. 92, 1995, pages 3214-3218, XP002219719 * See page 3215 (Crystallization of CPR) *</p>	1-52
P,X	<p>SHEWCHUK: "Structure of the Tie2 RTK domain: Self-inhibition by the nucleotide binding loop, activation loop, and C-terminal tail" STRUCTURE, vol. 8, November 2000 (2000-11), pages 1105-1113, XP001115087 * See the whole document; corresponding deposition at PDB (= 1FVR), release date 20-Sept-2001) *</p>	<p>1-5, 7-14, 17-25, 27-46, 48-52</p>

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# INTERNATIONAL SEARCH REPORT

Inte      tal Application No  
PCT/JS 01/27486

## C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
E	<p>WO 01 72778 A (BASF AKTIENGESELLSCHAFT)  4 October 2001 (2001-10-04)  * See SEQ.ID.No 1 (= SEQ.ID.No 2 / APPL)  and SEQ.ID.NO 2 (= 99.8 % of SEQ.ID.No 4 /  APPL -&gt; 7-323:11-327; i.e. except spacer,  and -RNL- (-RDL-/APPL) about position  170); p. 9ff and pp. 45-54 *</p> <p>-----</p>	<p>28-30,  34-41</p>



# INTERNATIONAL SEARCH REPORT

Information on patent family members

International Application No

PCT/US 01/27486

Patent document cited in search report		Publication date		Patent family member(s)	Publication date
WO 9513387	A	18-05-1995	AU	8143094 A	29-05-1995
			WO	9513387 A1	18-05-1995
WO 0172778	A	04-10-2001	AU	8726801 A	08-10-2001
			WO	0172778 A2	04-10-2001

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